2021-2030 White Paper for the Physics Division of National Center for Theoretical Sciences (NCTS-Physics)

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Introduction and Summary

This white paper represents a community effort to draw a roadmap for NCTS for the next decade (2021-2030) even though it is almost an impossible task.

During this exercise, we ask ourselves where we want to be research-wise ten years from now and how we can get there. The first thing we realize is that no matter where we decide to go, we should go together as a community. Because we believe if we want to have more great scientists in ten years, then the best strategy is to attract more and more people interested in doing science such that good scientists will emerge. We believe this approach will eventually lead to better results than investing exclusively on a few elite teams since the beginning. So the purpose of this white paper is to paint a future that is interesting enough to attract our community members to take this journey together.

Of course, we also realize that different members of the community have different needs. So we try to assess, whenever possible, existing research teams that are (A) internationally competitive already, (B) having the potential to do well with sufficient support, or (C) in the early stage but cannot afford to be left out. In the cases of (B) and (C), required resources and manpower can be addressed. It is our goal that the resources of NCTS can gradually move (C) teams to (B), (B) to (A), and make (A) teams even better.

About addressing the needs of manpower in the identified research areas, currently NCTS does not have its own faculty positions. However, we wish this document which provides a global view of the manpower issue could be a useful reference for hirings for institutes in Taiwan. It is also recommended that NCTS forms partnerships with those institutes to address the manpower issue.

Another pressing issue is the coordination of the mid- and large-scale computation resources. As computation, together with the surge of AI and machine learning, becomes more and more important in science, an expert team of user representatives to work with National Center for High-Performance Computing and related parties to work out a sustainable and scalable solution is critical and pressing.

Finally, as the boundary of each subfield expands, overlap among subfields becomes a norm. However, cross talk among subfields takes some efforts to overcome the initial barrier. NCTS is in a perfect position to help this synergy to happen.

Below are some general recommendations rephrasing the points mentioned above. Please refer to the writings contributed by individual thematic groups (TG's) for many more specific recommendations.

General Recommendations:

(1) **The role of NCTS should be to encourage more and more people interested in theoretical physics and help to provide a friendly environment to lower the barrier to participate in research. The hope is that by broadening the base of the research community, the chance for talents of exceptional capability to emerge is also increased.**

(2) **Teams that are well poised to tackle important problems and bring the community forward together are identified. Helping them to grow within NCTS and beyond is important.**

(3) **Manpower issues identified in this document are fundamental to the development of the future Taiwanese theoretical physics community. NCTS is encouraged to form strategic partnerships with institutes in Taiwan to further address these issues.**

(4) **To meet the increasing demand on high performance computation in different subfields, a team to work with National Center for High-Performance Computing (NCHC) and related parties to form a sustainable and scalable solution is critical.**

(5) **There are several topics that are interdisciplinary in nature, such as machine learning, quantum computation, information and devices, neutrino physics, dark matter, black hole and cosmology. They involve solid state, nuclear, high energy, astrophysics, information theory and so on. It is important to have a broad reach to the community while managing activities of those topics.**

Below we provide a brief introduction to NCTS-Physics then present the TG's contributions to the white paper.

A Brief Introduction to NCTS-Physics

Mission Statement: Focusing on team building and making NCTS an incubator to help young people succeed

Goals: National Center for Theoretical Sciences Physics Division (NCTS-Physics) has the dual goals of

(1) Becoming an academic exchange platform to serve Taiwan's theoretical physics community,

(2) Become a center of excellence in research.

Since its establishment in National Tsinghua University in 1997, the primary goal of NCTS-Physics was becoming a service platform. Resources were more evenly distributed to benefit the whole Taiwanese theoretical physics community. In 2015, a reorganization took place to focus the funding to transform NCTS-Physics to a center of excellence. To avoid being marginalized under the trend of globalization and the rise of China, this move had its strategic significance. However, an unexpected consequence was that a sense of community was lost for people outside of the center. Therefore, after NCTS-Physics moved to National Taiwan University in 2021, how to achieve the two goals of being a center of excellence and an excellent service platform at the same time has become the focus of the center's operation.

An example that pursues excellence and service simultaneously is the teamwork of cyclists in the Tour de France. In this sport, a team of cyclists are moving together and covering each other by taking turns to provide a windshield for the rest of the team. Then near the end of the race, the strongest cyclist breaks out the group and rushes to the end. In this collaboration, everyone benefits---the strongest member of the team enjoys the help from the rest of the team to block the wind along the way, while the rest of the team benefits from keeping up with the strongest member.

Our other important mission is to make NCTS an incubator to help young people to succeed. It is not a secret that heroes of theoretical physics typically have done their most important work when they were quite young. By channeling the main resources to young people, including, of course, students, we can probably reverse the decline of students going into theoretical physics.

*Therefore, our mission is to focus on **team building** to make NCTS an incubator to **help young people to succeed**.*

Strategy: The following is our strategy.

Team Building:
NCTS should focus on *building* and *serving* the teams, which are the most important part of the NCTS operation. The teams are identified by reviewing the past achievements of each field in the past decade and anticipating what the future might look like in the decade ahead to

(a) identify teams in Taiwan that are internationally competitive in fields that are important in the next decade

(b) identify fields that are important for the next decade and Taiwan has the potential to do well with sufficient support or cannot afford to be left out

These teams are called thematic groups (TG's) and they will be led by center scientists (CS's). While TG's are identifying bigger trends in the fields, smaller and emerging trends can be investigated within TG's or forming seed programs called "Program X".

In order to improve efficiency, we have set up several Hubs based on the geographical distribution of CS's and members of the TG's. The Hubs should have their own secretary support and have postdocs stationed around the key members of the TG's to maximize teamwork.

In addition to face-to-face communication, it is also very important to help members to communicate or conduct joint seminars through the internet to achieve efficient collective motion.

Become an incubator to help young people succeed:
We would like to channel the funds to young people. Therefore, we hope to reduce the average age of center scientists to 30's or 40's. The meetings that NCTS organizes/sponsors should make sure that young people enjoy a significant portion of the spotlight.

In cultivating students, our challenges are

(a) the number of students entering theoretical physics is decreasing over the years
(b) the number of female students is low
(c) students do not consider entering Ph. D. program in Taiwan a top career choice. However, the number of students studying abroad (not limited to physics students) is also declining. (Taiwan was ranked among the top two sources of foreign students in the US from 1950-1989. Then it was ranked 7th in the world, after Vietnam, in 2018.)

Fortunately, NCTS can serve as a vehicle to reverse these trends by promoting female scientists, providing shared courses and holding various activities such as theory Hackathon, theory Oscars awards, and so on to convey the fun and beauty of working in theoretical physics.

We will also target rising stars and provide Distinguished Junior Lectureship or short-termed focused programs to be led by those young talents *before* they become famous to establish valuable long term relationships.

Conclusion:

We want to build NCTS as a center of excellence and a platform that serves the entire community at the same time. We will focus on team building and make NCTS an incubator to help young people to succeed. If NCTS can be successful in team building to unleash the power of collaboration, then it will open the window of boundless opportunities. NCTS would not only help people of the same disciples to work together, but also people of different disciplines to tackle problems of much larger scope. We can foresee NCTS plays an important role in problems that are important for human civilization, such as artificial intelligence, climate change and sustainability, space exploration, and so on. We have seen a very bright future for NCTS and let us work together to make it happen.

TG1: Quantum Information and Quantum Computing

Recent development of quantum technology has sparked a new wave of the scientific and industrial revolution, including the pursuit for quantum computing (QC), communication, new perspectives of information science, artificial intelligence, and novel methodology for many interdisciplinary fields such as quantum chemistry, biophysics, drug, and material design, and finance. As the commercial quantum computing services (e.g., IBM, Google, etc.) emerge in the market, the quantum experiences start to become reality for these communities. Recently, Google has claimed the advent of quantum supremacy, that is, the quantum machine has been demonstrated to overpower the classical means on certain specific problems.

It is still expected, however, that a long journey remains ahead to practical quantum machinery that really helps solve important problems. The relevant research in these areas in Taiwan is still in its infancy stage. It is a role and even an obligation that NCTS should take to nurture this emerging and promising field, help the community, lead the trends in the fundamental studies, serve as a bridge between theorists and on-going experiments in Taiwan, and facilitate international collaborations.

The interrelations between relevant subjects and growing interests can be summarized by the three-circle figure in Fig. 1. The main scopes of the field include the three categories that are closely connected and overlapped.

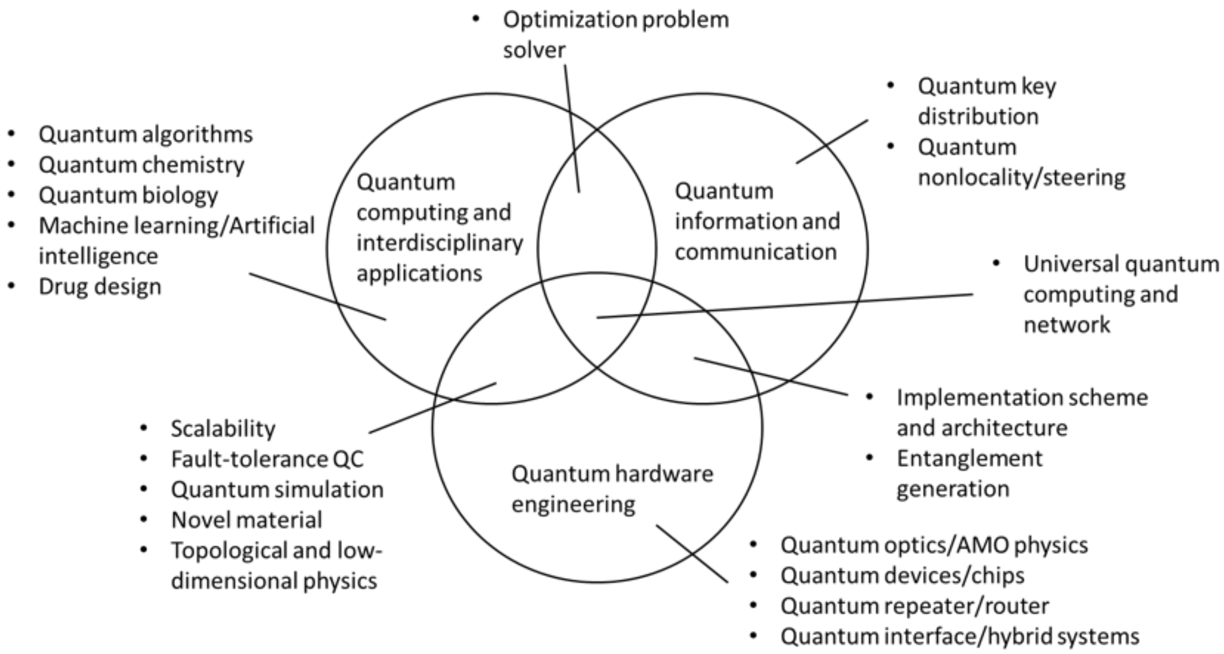

FIG. 1: The interrelations between relevant subjects and growing interests in Quantum Computation and Quantum Information.

As the whole industry is too broad to be focused, here we propose to work on the following areas by considering the experience and expertise of the theoretical physicists in Taiwan:

TG1.1: Quantum Computing and Interdisciplinary Applications

Previous Milestones: Quantum computing (QC) is an entirely new paradigm of computation that promises to solve some of the problems that are intractable on classical supercomputers. In the past few years, we have witnessed a great surge in global funding for basic research and engineering of quantum computing technologies. In 2019, Google claimed to demonstrate quantum supremacy, where a 53-qubit superconducting quantum computer outperformed a classical supercomputer in random number generation [1.1.1]. Later in 2020, a further demonstration of quantum supremacy using an optical circuit (quantum computer prototype), Jiuzhang, performed a quantum computation called "Gaussian boson sampling" in 200 seconds, 100 trillion times faster than a supercomputer could [1.1.2]. Furthermore, IBM has announced its QC hardware and software development roadmap pointing to massive increase in both qubit number and the speed of quantum circuits in the next 5 years [1.1.3]. Together with improvements to quantum software, this in turn will tremendously speed up useful quantum applications.

Towards a viable technology: For quantum computing to become a viable technology, the following general significant breakthroughs ought to happen: (1) revolutionary quantum hardware that is scalable and could reach error rates less than 10^{-3} and circuit depth greater than 10000 gates (2) multiple applications of quantum computing to real-world problems that demonstrate true quantum advantage, and (3) a clear path towards fault-tolerant quantum computation. These challenges are extremely difficult to overcome; however, the stakes are also extremely high.

Important directions in the next decade: In the area of Quantum Computing and Interdisciplinary Applications, we have identified the following subjects as being important in the next decades:

(1) High-fidelity and robust control: To realize practical quantum computation, a set of high-fidelity universal quantum gates robust against noise in the qubit system is prerequisite. Constructing control pulses to operate quantum gates which meet this requirement is an important issue. In most of the robust control methods, noise is assumed to be quasi-static, i.e., is time-independent within the gate operation time but can vary between different gates. But this quasi-static-noise (QSN) assumption is not always valid. Therefore, one needs to develop a robust control method that goes beyond the QSN domain, and implement it, taking into account the real-world quantum-device noise scenarios for quantum computation, to construct high-fidelity quantum gates with fidelities enabling large-scale fault-tolerant quantum computation [1.1.4].

(2) Quantum circuit speedup and noise mitigation: We are now in the so-called noisy intermediate-scale quantum (NISQ) era with quantum computers composed of hundreds of noisy qubits, i.e. qubits that are not error-corrected, and therefore perform imperfect operations in a limited coherence time [1.1.5]. The NISQ algorithm solution for noisy and imperfect quantum gates and measurements is to work with a small number of qubits and low circuit depth. Algorithmic research for improving the efficiency of quantum circuits – circuit compilation, efficient hardware-specific quantum gates… etc. are also important for simulation/experiments run on NISQ machines [1.1.6]. Noise characterization and mitigation methods for modern NISQ hardware are also crucial to obtain sensible results.

(3) Error-correction codes and fault-tolerant quantum computation: A quantum computer with error correction is required for large scale quantum computing. Investigating what really "makes" or "constitutes" quantum error correction (QEC) is an important problem [1.1.7]. The aim is to review current such theories, and see if it's possible to elaborate on, modify or improve the existing ones, or even propose a new model for error correction. Surface/topological codes are stabilizer codes which utilize topological properties such that the stabilizer group can be easily found, and such codes can be scaled up with relative ease, so the surface code is one of the most promising quantum error correction schemes. [1.1.8] Efficient hardware implementations of the surface code [1.1.8] or other novel QEC codes [1.1.9] on superconducting qubit systems, semiconductor spin qubit systems and other promising qubit systems towards fault-tolerant quantum computation are important problems to investigate.

(4) Quantum machine learning (QML): Quantum computing and machine learning (the core of contemporary artificial intelligence) are emerging and promising technologies that would have a major impact on human life and society in the future. QML is to investigate the extent to which these two fields can indeed learn interactively and benefit from each other, that is, to explore the interaction between quantum computing and machine learning, and study how to use the results and technologies of one field to solve problems in another field [1.1.10,1.1.11]. In particular, focus will be put on algorithms and applications that can be implemented in the current and near-term NISQ machines [1.1.12,1.1.13]. An initial step is to understand the theoretical foundations of classical machine learning and artificial intelligence, and then generalize to the quantum correspondence. Then provide theoretical evidence and provable system setups for quantum machine intelligence. Interesting subjects and questions are as follows. How much computational resources (e.g., number of qubits and depths) are required to accomplish certain quantum machine learning tasks? How robust is the quantum machine learning algorithm to the quantum computer (e.g., gate fidelity etc.)? What is the accuracy that the quantum machine learning algorithm can achieve? How many instances are needed by the quantum machine learning algorithms in the training phase?

(5) Quantum simulation and quantum chemistry: Quantum computer systems provide excellent platforms for conducting experiments to investigate interesting quantum physics and phenomena, and to verify proposed quantum theory and protocols. They are also excellent platforms for performing simulations to simulate other quantum systems [1.1.14]. The variational quantum circuit approach with tunable parameters optimized in an iterative manner by a classical computer is a hybrid quantum-classical approach which leverages the strengths of quantum and classical computation. It has proven successful in the high accuracy calculation of the electronic structure in small molecular systems. This promising computational tool enables the use of a complex scheme to capture the electronic correlations in molecular systems [1.1.15,1.1.16]. The next step is to investigate systems with large size and/or with complicated interactions (e.g., electronic correlations). Another question is whether quantum computing can be used to study the correlation effects in solid state systems, i.e., systems with periodicity, as well as to strongly correlated systems. These studies are important to materials science and new drug design.

(6) Quantum finance and optimization problems: Quantum finance and optimization are interdisciplinary research fields that apply theories and methods developed in quantum computing in order to solve problems in finance and optimization [1.1.17,1.1.18,1.1.19]. Many problems can be formulated as optimization problems by finding decisions or making actions that result in the best possible outcome for a given goal subject to some constraints, for example, finding the best supply-chain route for delivery, determining the best investment strategy for a portfolio of assets, or increasing productivity with a number of fixed resources in operations. In addition to the problems that can be expressed as optimization problems, other problems in finance, such as auction, option pricing, risk management, automated portfolio management, algorithmic trading, risk assessment, fraud detection can be potentially treated by quantum machine learning or quantum Monte Carlo methods [1.1.17,1.1.18,1.1.19]. Interests and emphases will be focused on tasks which are particularly hard for classical computers, but could find a natural formulation using quantum methods or quantum inspired algorithms.

Strengths and opportunities for Taiwan:

(a) Talents in Taiwan:

The following researchers are talents in this field in Taiwan: Hsi-Sheng Goan (NTU), Yuan-Chung Cheng (NTU-Chem), Hao-Chung Cheng (NTU-EE), Yufeng Jane Tseng (NTU-CC), Jyh-Pin Chou (NCUE), Ching-Ray Chang (NTU), Ying-Jer Kao (NTU), Sy-Yen Kuo (NTUEE), Yen-Huan Li, (NTUCS), Tsan-Chuen Leung (CCU), Yao-Hsin Chou (NCNUCS), Chia-Mu Yu (NCTUIMF), Li-Yi Hsu (CYCU), Tsung-Wei Huang (CYCU-CS), Chih-Yu Chen (CYUU), Jie-Hong Jiang (NTU-EE), Chien-Mo Li (NTU-EE), Shih-Hao Hung (NTU-CC), Shih-Wei Liao (NTU-CC), Shu-Yu Kuo (NCHU-CC), Daw-Wei Wang (NTHU), Yueh-Nan Chen (NCKU), Ray-Kuang Lee (NTHU-EE), Guin-Dar Lin (NTU), Chiao-Hsuan Wang (NTU), Ching-Yi Lai (NYCU), Che-Ming Li (NCKU-ES), Chung-Yu Mou (NTHU), Min-Hsiu Hsieh (Hon-Hai)

(b) Recommended Strategy and teams to watch:

We have the following achievements on the above topics in the recent years:

We have made substantial contributions to the area of high-fidelity and robust control for quantum gate operations for various promising quantum computing systems, ranging from superconducting qubits, nitrogen-vacancy centers in diamond, trapped ions, silicon-based donor-impurity as well as quantum-dot spin-qubit systems, etc. We have proposed a scheme to accelerate the speed and performance of quantum circuits. We have demonstrated that it is possible to efficiently detect certain faults or errors in a quantum circuit. We have presented the first proof-of-principle demonstration of deep reinforcement learning using variational quantum circuits. This work has also demonstrated quantum advantage in terms of less memory consumption and the reduction of model parameters. We have also demonstrated that choosing an appropriate basis set of spin orbitals in applying quantum computing to computational chemistry. Our calculations produce accurate structural optimization of selected molecules (H_2, LiH, and H_2O) at low computational cost and the results of H_2 and LiH vibrational frequencies are in excellent agreement with experimental data.

We also identify here some research topics that are important for the next decade, which Taiwan has just gotten momentum in investigating upon. For example, research topics like quantum error correction is essential for large-scale quantum computation, and quantum finance and optimization problems are research topics that quantum computing can potentially provide significant speedup and substantial impact on.

Overall, the research fields in this area are rapidly evolving and require cross-disciplinary and interdisciplinary efforts. For example, quantum finance, new drug design, and biologic and chemical reactions, etc., often require deep domain specific knowledge and thus the collaboration between quantum algorithmic and respective disciplinary experts is essential in order to be able to increase the impact of quantum algorithms and harness the computational potential of the NISQ machines.

The identified research topics in TG1.1 are important for the next decade and cannot afford to be left out.

We will hold seminars, discussion meetings, short courses, school and workshops/conferences to encourage more and more people to get interested in and get opportunities and channels to learn and investigate the research topics. Through bringing the community forward together to form a critical mass, we believe that Taiwan has the potential to do well with sufficient support in these interesting research areas. We list below the recommended subjects and team to watch for each identified research field.

Recommended subjects:

(1) High-fidelity and robust control

- Characterizing decoherence and noise sources of practical quantum computer devices
- New robust control schemes
- Constructing high-fidelity quantum gates in the presence of realistic noise and decoherence
- Constructing robust quantum gate operations using machine learning techniques

Team: HS Goan, CH Wang, GD Lin

Our overall research performance along this broad research direction indicates that we are in state (B), having the potential to do well with sufficient support.

(2) Quantum circuit speedup and noise mitigation:

- Development of cross-platform quantum software that integrates diverse tools from modern quantum ecosystems
- Algorithmic research for improving the efficiency of quantum circuits – circuit compilation, efficient hardware-specific quantum gates… etc.
- Noise characterization and mitigation methods for modern quantum hardware

Team: JH Jiang, CM Li, SW Liao, SH Hung, SY Kuo, YH Li, YH Chou, YN Chen, YC Cheng, MH Hsieh

Our overall research performance along this broad research direction indicates that we are in state (B), having the potential to do well with sufficient support.

(3) Error-correction codes and fault-tolerant quantum computation:

- Theories for novel quantum devices and collaborations with experimental groups to develop new qubit systems
- Efficient hardware implementations of the surface code or other existing QEC codes
- Novel QEC codes
- Hardware implementations of QEC codes towards fault-tolerant quantum computation

Team: CY Lai, MH Hsieh, HS Goan, CH Wang

Our overall research performance along this broad research direction indicates that we are in state (C) cannot afford to be left out. As more researchers are working on this important topic, in turn bringing more students and postdocs into the field, we may potentially move to state (B) in a few years.

(4) Quantum machine learning

- Machine learning for simulating and predicting properties and phenomena of quantum systems
- Hybrid quantum-classical algorithms for solving quantum problems in NISD systems
- Efficient schemes for encoding classical data into quantum states
- Efficient schemes for extracting information from quantum states
- Understanding the theoretical foundations of classical machine learning and artificial intelligence, and then the generalization to the quantum correspondence
- Computational resource (e.g., number of qubits and depths), training instances required to accomplish certain quantum machine learning tasks
- Robustness and accuracy of quantum machine learning algorithms
- Neural network with hybrid system of quantum and classical components.
- Variational quantum circuits with adjustable encoding method

Team: HC Cheng, MH Hsieh, HS Goan, YJ Kao, DW Wang, RK Lee, SH Hung, SW Liao

Our overall research performance along this broad research direction indicates that we are in state (B), having the potential to do well with sufficient support.

(5) Quantum simulation and quantum chemistry

- Hybrid quantum-classical algorithms for solving quantum problems in NISD systems
- Quantum simulations of dynamics of complex systems for fundamental physical and chemical research
- Quantum simulations of molecular energy structure of new materials
- Quantum simulation of chemical reaction and new drug design

Team: YC Cheng, YF Tseng, JP Chou, HS Goan, CW Hwang, YN Chen, CM Li, CY Mou

Our overall research performance along this broad research direction indicates that we are in state (B), having the potential to do well with sufficient support.

(6) Quantum finance and optimization problems

- Classically computationally challenging problems: active investment management, portfolio optimization, option pricing, risk assessment and management, market trading, fraud detection, etc.
- Methodology in quantum finance
- Quantum inspired algorithms for finance
- Convex optimization problems
- Discrete Problems: Variational quantum eigensolver (VQE) and quantum approximate optimization algorithm (QAOA).
- Combinatorial optimization problems: Quadratic unconstrained binary optimization (QUBO) using quantum annealing and quantum inspired digital annealing

Team: CR Chang, TW Huang, CY Chen, YH Chou, CM Yu, SY Kuo, SH Hung, TC Leung

Our overall research performance along this broad research direction indicates that we are in state (C) cannot afford to be left out. At the moment, most local researchers are working on problems using quantum inspired algorithms or QUBO problems using quantum or digital annealing methods. So we may start by first encouraging the hiring of principal investigators and postdoctoral researchers specializing in the other corresponding subjects in quantum finance.

(c) Recommendations on future critical hiring:

New hires with expertise and experience at the hardware and software interface are strongly recommended as they can to work on (i)-(iii), where significant contribution can still be made. New hires working on the interdisciplinary real-world application of quantum computing are also strongly desirable, especially on quantum finance, new material simulation and new drug design.

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TG1.2: Quantum Physics and Quantum Engineering

Important directions in the next decade:

There are many promising platforms to study quantum physics and quantum engineering, from atom-molecular-optics (AMO), solid-state, NMR, to superconducting systems. In particular, the studies on light-matter interaction is the key scenario with the ability to prepare, manipulate, and detect the resulting quantum outcomes. However, interdisciplinary backgrounds are naturally needed for the varieties in different platforms. Quantum optics and optical spectroscopy are at the heart of the advances in experimental quantum science. In Taiwan, we have colleagues working on photonic quantum state generation and detection, quantum memory based on light-atom interaction, circuit-QED with Josephson junctions, quantum gases in Bose-Einstein condensates, precision spectroscopy with atoms and ions, and quantum metrology for the gravitational wave detectors. In relation to quantum physics and quantum engineering, we have identified the following subjects as being important in the next decades in this theory space:

(1) Quantum Optics, with the connection to quantum information processing (TG 1.3);

(2) Quantum Gases, with the connection to many-body physics and quantum simulation (TG 1.1 and TG 3.2);

(3) Cavity-and Circuit-QED, and Quantum Interface, with the connection to quantum computing (TG 1.1);

(4) Quantum assisted High Precision Measurements, and Quantum Metrology for the Gravitational Wave Detectors (TG 2.3).

(1) Quantum Optics:

In general, the studies on the interaction between photon and matter belong to this sub-field. For the photon part, it includes the generation of single-photon, entangled photon pairs, squeezed states, optical cat states, cluster states, multi-parties, and macroscopic states. For the matter, the possible platforms include atomic systems, nonlinear crystals, optomechanical systems, micro-resonators, Josephson junctions, quantum dots, NV-centered diamonds, single atom and ion. The phenomena to be explored are nonlinear dynamics, collective excitation, soliton/vortex formations, optomechanical coupling between phonons and optical photons, superradiance, and storage/retrieval of quantum information. Utilizing the tools developed for quantum optics, we are now able to control individual atomic quantum systems, making these a natural choice for implementing structures for quantum information processing and simulation [1.2.1]. The connection and application of Quantum Optics range from the test of foundation of quantum mechanics (with TG 1.3), the building block for quantum information processing, quantum computing, and quantum communication (with TG 1.1, 1.2) [1.2.2].

(2) Quantum Gases:

Atoms are the ideal quantum system since they are nearly non-interacting and, more importantly, are indistinguishable. The physical systems include Bose-Einstein condensates (BECs), quantum Fermi gases, polar molecules, Rydberg-dressed BECs, and exciton polaritons, with emphasis on the exotic phenomena due to the intrinsic two/three-bodies interaction. Related nonlinear dynamics, collective excitation, manipulation, spontaneous synchronization in the quantum domain and collaboration with experimental groups are all of high interest in the direction of research agenda. One main application of quantum gases is to provide the platform for quantum simulation. In particular, synthetic gauge fields with spin-orbital coupling, topological states, non-equilibrium dynamics, quantum spontaneous synchronization, Abelian/non-Abelian gauge potentials. Supersolidity, Anderson localization, quantum turbulence, and polariton formations in quantum gases are actively investigated for many-body physics and quantum simulations. The studies on Quantum Gases can synergy with strong correlated systems (TG 3.2) and complex systems (TG 4) [1.2.3].

(3) Cavity-and Circuit-QED and Quantum Interface:

A different approach to exploring solid-state devices with quantum optical systems is being pursued in the field of "atomtronics". Potentially, hybrid quantum systems could lead to such advances. By leveraging the fabrication of Josephson junctions, as the artificial atoms, in the circuit-QED setting, gate-based quantum computing and related input-output quantum interfaces are the practical applications. Emerging applications and challenges to be addressed include controlling the decoherence, scale-up complexity, quantum interface among different platforms, and robust control theory. Joint activities with TG 1.1 on quantum simulations arise naturally [1.2.4].

(4) Quantum assisted High Precision Measurements, and Quantum Metrology:

The standard quantum limit (SQL), but not yet the Heisenberg limit, sets the lower bound in the current precision measurements. It is possible to approach the Heisenberg limit by using specially prepared quantum states with well-chosen quantum mechanical correlations. Possible choices include entangled states or spin-squeezed states. Currently, the astrophysical reach of current and future ground-based gravitational-wave detectors is mostly limited by quantum noise, induced by vacuum fluctuations entering the detector output port. The replacement of this ordinary vacuum field with a squeezed vacuum field has proven to be an effective strategy to mitigate such quantum noise and it is currently used in advanced detectors. However, how to overcome the fragile nature of quantum squeezed vacuum is a critical and expectable issue in these quantum assisted high precision measurements. Quantum sensors and the quantum-enhanced spectroscopy should provide the quantum assisted high precision measurement for atomic clocks, molecular spectroscopy, and advanced gravitational-wave detectors, which can synergize with TG 2.3 and TG 4 [1.2.6].

Strengths and opportunities for Taiwan:

(a) Talents in Taiwan:

We already have several PIs working on atomic systems, nonlinear crystals, Josephson junctions, quantum dots, NV-centered diamonds, single atom and ion, and X-ray quantum optics. Active groups include AS, NTU, NTHU, NCU, NCHU, NCKU. The following researchers are talents in this field in Taiwan: Hsi-Sheng Goan (NTU), Guin-Dar Lin (NTU), Ying-Cheng Chen (AS), Yi-Ju Lin (AS), Ming-S, Ite A. Yu (NTHU), Daw-Wei Wang (NTHU), Yueh-Nan Chen (NCKU), Ray-Kuang Lee (NTHU), Io-Chun Hoi (NTHU), Shih-Kuang Tung (NTHU), Yi-Hsin Chen (NSYSU), Watson Kuo (NCHU), Yen-Hsiang Lin (NTHU), Shin-Tza Wu (CCU), Wente Liao (NCU), Wei-Min Zhang (NCKU), Junyi Wu (TKU), Chung-Yu Mou (NTHU)

(b) Recommended Strategy and Teams to Watch:

(1) For Quantum Optics, possible subjects to pursue are optomechanical systems and micro-resonators.

(2) For Quantum Gases: There are strong overlappings and collaborations among the PIs working in this subject and strong-correlated condensed matter physics (TG 3.2), as well as quantum simulations (TG 1.1). Active groups include AS, NTHU, NTNU, NYCU, NCKU.

(3) Cavity-and Circuit-QED and Quantum Interface: It should be good to have people working in this interdisciplinary problem, in particular with a solid theoretical training. Active groups include AS, NTU, NTHU, NCHU.

(4) Quantum assisted High Precision Measurements, and Quantum Metrology: Approaches from information-oriented should be useful to design new quantum metrology. Joint activities with TG 1.3 on quantum information science should be addressed. Moreover, the application of quantum metrology to the gravitational wave detectors also emerges with the targets on black-hole physics, cosmology , and dark matter/energy searches (TG 2.3). Active groups include AS, NTHU, NCU.

(c) Recommendations for NCTS:

Young talents, who are not only with a strong background in theory, but also familiar with experiments.

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TG1.3: Quantum information and communication

Quantum information science (QIS), despite being developed for nearly thirty years, is still a rapidly evolving research frontier that has drawn an increasing level of interest. In a nutshell, it is the science of quantum systems and that of information theory where the information carrier is assumed to be of quantum origin. Throughout the years, it has helped us to understand how fundamental quantum mechanical principles can be harnessed to improve the storage, processing, and communication of information.

Important directions in the next decade

(1) Information-theoretic approaches to physics

A byproduct of the development of quantum information theory is an increasing focus towards a more information-theoretic approach to physics, an effort that could be traced back, at least to work of Landauer [1.3.1], Jaynes [1.3.2], among others. More recently, the so-called black hole information paradox [1.3.3] and its resolutions have led to a better understanding of black hole physics, which is of interest in TG2.2 and TG2.3 as well, even though there is still no unanimously accepted theory of quantum gravity. Another notable example of this kind is a consolidated effort initiated by the quantum information community several years ago to understand the thermodynamics of quantum systems [1.3.4]. Some distinctive features of such an approach are the employment of entropic quantities and/ or the utilization of resource theories [1.3.5] to determine what's allowed or forbidden in physical theory. In recent years, there's also an increasing effort of using such an approach to understand how well a quantum system can be used as a time-keeping device.

(2) Quantum cryptography and its security proofs

Quantum cryptography [1.3.6] is an interdisciplinary field that aims to understand the role of quantum effects in cryptography. On the one hand, quantum adversaries can break most currently deployed public-key cryptography by Shor's algorithm. Whereas on the other, the power of quantum allows us to bypass classical impossibility, such as, enabling secure communication with information-theoretic security and opening the venue of cryptography with quantum functionalities (such as the encryption of quantum data to allow for blind computation). Due to its interdisciplinary nature, the study of quantum cryptography often combines state-of-the-art techniques from cryptography, quantum physics, complexity theory, and information theory. In turn, quantum cryptography also provides a rich context to develop deep insights and new techniques to advance the study of these fields.

(3) Quantum effects in biological, relativistic, and other macroscopic or large-scale systems

The existence (and observation) of quantum effects in biological [1.3.7] or other large-scale physical systems [1.3.8] has always been a subject of heated debate. In part, this is because well-controlled experiments on such systems are extremely challenging. In fact, even arriving at a good theoretical model for such systems is far from trivial. Nonetheless, our ignorance of such systems is suggestive that new physics can be learned from a better understanding of the quantum effects present or their lacking in such systems. (In this regard, synergy with TG4.2 will be beneficial.) On the other hand, a solid understanding of how quantum effects are modified in a relativistic setting [1.3.9], or under a different spacetime topology is clearly also of paramount importance. This is of interest not only from a fundamental viewpoint but also relevant to the implementation of quantum technologies at large scales, such as between ground-based stations and satellites.

(4) Quantum foundations, decoherence dynamics, and applications in quantum information

Quantum foundations (see, e.g., [1.3.10, 1.3.11, 1.3.12]) represent a very broad research program that sits at the intersection of quantum physics, mathematics, and philosophy. The general aims are to (1) establish a more intuitive understanding of the mathematical foundations of quantum theory, (2) provide an interpretation of what the various notions involved in quantum theory mean, (3) understand in a broad context how quantum theory differs from a general physical theory and what constitutes a genuine quantum effect, (4) better understand how and why quantum effects get suppressed in daily observations. Of course, the last of these aims is closely to the study of the decoherence dynamics [1.3.13] of various physical systems and models.

Over the years, research that originated in quantum foundations has not only led to a better understanding of the theory but also useful applications in the field of quantum information itself. Notable examples of this include the development of quantum key distribution protocols [1.3.14] and quantum random number generation protocols [1.3.15] that are secure even against post-quantum adversaries, as well as the robust certification of quantum devices with minimal assumptions (see, e.g., [1.3.16]).

Strength and opportunities in Taiwan

(a) Talents in Taiwan

The following researchers are talents in this field in Taiwan: The core members of TG1.3 [Guang-Yin Chen (NCHU), Yueh-Nan Chen (NCKU), Chung-Hsien Chou (NCKU), Kai-Min Chung (IIS, Academia Sinica), Li-Yi Hsu (CYCU), Ching-Yi Lai (ICE, NYCU), Che-Ming Li (ES, NCKU), Yeong-Cherng Liang (NCKU)], as well as Ching-Hsu Chen (NCYU), Hong-Bin Chen (ES, NCKU), Yuan-Chung Cheng (Chemistry, NTU), Hsi-Sheng Goan (NTU), Chi-Chuan Hwang (ES, NCKU), Tzone-Lih Hwang (CSIE, NCKU), Feng-Li Lin (NTNU), Han-Hsuan Lin (CS, NTHU), Shih-Yuin Lin (NCUE), Chia-Wei Tsai (CSIE, NTTU), Jun-Yi Wu (TKU), Zheng-Yao Su (NHPC)

(b) Recommended strategy and teams to watch

We have the following achievements on the above topics in recent years:

(1) Information-theoretic approaches to physics

In 2015, we have proposed an operational approach to time by defining a minimal notion of a quantum clock and describing how one can use an operational task, i.e., a game to quantify how well a physical system can be used as a time-keeping device without reference to any background time (arXiv 2015). This has since inspired a series of work studying autonomous quantum clocks and the cost of measuring time. Meanwhile, we proposed the notion of information flux for open quantum systems and used it to analyze the non-Markovianity of such systems (PRA 2017). We also explored correction to entropic uncertainty relation based on generalized uncertainty principles (MPLA, 2017). In a very different context, we have used Holevo information to show that black hole microstates are indistinguishable from thermal states by measuring over a small region but perfectly distinguishable over a region with its size comparable to the whole system (PRL 2018).

Our overall research performance along this broad research direction indicates that we are in state (C) cannot afford to be left out. At the moment, we have too few people working in this rapidly evolving research direction. As such, we should start by first encouraging the hiring of principal investigators and postdoctoral researchers specializing in the corresponding topics.

Recommended subjects:

-- Information-theoretic approaches to quantum thermodynamics

-- Information-theoretic approaches to open-system dynamics

-- Information-theoretic approaches to the study of quantum systems as a time-keeping device

-- Blackhole information paradox

Team: HB Chen, GY Chen, YN Chen, YC Liang, FL Lin

(2) Quantum cryptography and its security proofs

We have been making contributions to the field of quantum cryptography since nearly two decades ago. For example, we proposed tomographic quantum key distribution protocols (PRA 2003) and showed that the optimality of so-called square-root measurements is unwarranted in such protocols (PRA 2004). We have also proposed some other quantum key distribution protocols with their security analyzed (IEEE Trans. Dep. Sec. Comp. 2007, IET Inf. Sec. 2007). Moreover, we have proposed some versions of quantum secret-sharing protocols and/or analyzed the security of some such protocols (PRA 2003, PRA 2005, PRA 2008, IJMPC 2009, CJP 2010, IJTP 2012, QIP 2013, QIP 2014, etc.). In addition, we have proposed some quantum private comparison protocols (QIP2011, EPJD2011) and analyzed the security of so-called quantum secure direct communication protocols (Sci. China 2011, Opt. Comm. 2011, QIP 2014, etc.). More recently, we proved the possibility of general randomness amplification with non-signaling security (QIP'2017). We have also initiated the study of computational notions of quantum min-entropy (QCrypt'2017), given the first construction of a non-malleable extractor secure against quantum adversaries (Eurocrypt'2019), contributed to the studies of quantum private information retrieval (Eurocrypt'2019), practical randomness generation (QST 2019), and the security analysis in the quantum random oracle model (ITC'2020), etc.

Our overall research performance along this broad research direction indicates that we are in state (B), having the potential to do well with sufficient support. As this is, globally speaking, a fairly mature research area, we can do better by sending, on a regular basis, young local talents abroad to attend schools, etc. to receive advanced training.

Recommended subjects:

-- General security proof of quantum key distribution protocols

-- Blind quantum computation

-- Device-independent quantum cryptographic protocols

-- Quantum random number generations

Team: KM Chung, LY Hsu, TL Hwang, CY Lai, CM Li, FL Lin, HH Lin, YC Liang, CW Tsai

(3) Quantum effects in biological, relativistic, and other macroscopic or large-scale systems

We have introduced tools that enable efficient verification of quantum coherence and dynamics in the time domain, applicable to solid-state as well as biological systems (Sci. Rep. 2012). In 2013, we provided a review for the state-of-the-art of quantum biology in Nature Physics. Then, we proposed an analytical non-Markovian model to explain the origin of the long-lived coherence in pigment-protein complexes (PRE 2014). We further showed that quantum coherence plays a crucial role in enhancing the performance of biological quantum heat engines (PRE 2016) and that strong non-Markovianity is present in the radical pair model of magnetoreception (PRA 2016). More recently, we showed that an efficient quantum simulation of photosynthetic light-harvesting is possible (npj QI 2018). Meanwhile, we also investigated the coherent single surface-plasmon transport in a metal nanowire strongly coupled to two colloidal quantum dots (PRB 2011). In the relativistic setting, we have analyzed how quantum teleportation depends on the motion between moving detectors (PRD 2015). We have also investigated the entanglement dynamics between two Unruh-DeWitt detectors in various relativistic settings (PRD 2008, JHEP 2012, JHEP 2016, PRD 2018).

Our overall research performance along this broad research direction indicates that we are in state (B), having the potential to do well with sufficient support. For both quantum effects in biological systems and in relativistic settings, we already have good connections with international researchers. With sufficient support, these strong ties can be and should be maintained.

Recommended subjects:

-- Quantum effects in photosynthesis, avian compass, etc.

-- Possible quantum effects at the macroscopic scale

-- Possible quantum effects at the cosmological scale

-- Corrections of quantum effects in a relativistic setting

Team: GY Chen, HB Chen, YN Chen, YC Cheng, CS Chou, CC Hwang, CM Li, FL Lin, SY Lin

(4) Quantum foundations, decoherence dynamics, and applications in quantum information

We have started working on quantum foundations more than a decade ago. For example, already in 2008, we showed that all bipartite entangled states are capable of showing a subtle form of Bell-nonlocality that may be hidden (PRL 2008). In 2011, we wrote a review paper for Physics Reports on contextuality, nonlocality, and complementarity. We further showed that under the premise of a non-signaling world, a class of physical models purporting to explain the origin of Bell-nonlocal correlations is untenable (Nature Phys. 2012). More recently, by revisiting Wigner's friend paradox, we showed that a stronger no-go theorem could be established to illustrate the tension between quantum prediction and the absoluteness of events (Nature Phys. 2020). Moreover, we explored quantum Chesire cat and their connection with elements of reality (PLA 2020).

We have also contributed actively on how the observation of Bell-nonlocal correlation between (spatially-separated) measurement outcomes enables the certification of the preparation and measurement devices with minimal assumptions (PRL 2011, PRL 2013, PRL 2015, PRL 2016, PRR 2019, etc.), even without a shared reference frame (PRL 2010, Sci Rep 2012, PRA 2020). By considering a weaker form of such spatial correlations called EPR steering, which correspond to allowing more trust on a subset of the physical systems, we developed a novel formalism to explore such a phenomenon in situations involving multipartite quantum systems of high dimensionality (PRL 2015). More recently, we have also used EPR steering to characterize the number of classical nodes in quantum networks (PRL 2020).

Meanwhile, to understand the analogous correlations in time, we have made use of Leggett-Garg inequalities to distinguish quantum from classical transport through nanostructures (PRL 2010). We have also introduced the notion of temporal steering (PRA 2014) and used it, among others, to quantify non-Markovianity in the dynamics of physical systems (PRL 2016). For the analysis of dynamics, we have introduced a resource theory to describe quantum memories (PRX 2018). In addition, we introduced the framework of Hamiltonian-ensemble simulation to characterize the (non)-classicality of open-system dynamics (PRL 2018) and used it to quantify the nonclassicality of pure dephasing channels (Nature Commun. 2019).

We have also a long history of involvement in the studies of decoherence dynamics. For example, we have derived an exact mast equation to analyze the decoherence of two coupled harmonic oscillators in a general environment (PRE 2008). We have also presented a general theory of non-Markovian dynamics for an open system of non-interacting fermions/bosons linearly coupled to thermal environments of non-interacting fermions/bosons (PRL 2012). In particular, we have analyzed the non-Markovian dynamics for continuous-variable quantum channels (PRA 2007), for double-dot charge qubit (PRA 2008), for microcavity coupled to a waveguide (Opt. Exp. 2010), and for a nanocavity coupled to a coupled-resonator optical waveguide (PRA 2011). Besides, we have also studied non-Markovian complexity in the quantum to classical transition (Sci. Rep. 2015) and analyzed the decoherence from Majorana modes (NJP 2014 and PRB 2018).

Our overall research performance along this broad research direction indicates that we are in state (A)---international competitive already.

Recommended subjects:

-- General physical theories (GPT)

-- Bell-nonlocality, steering, device-independent and semi-device-independent quantum information

-- Causal structures and quantum correlations in time

-- The measurement problem and its resolution

-- Decoherence dynamics of physical systems

Team: CH Chen, HB Chen, YN Chen, CH Chou, KM Chung, HS Goan, LY Hsu, CM Li, YC Liang, ZY Su, JY Wu, WM Zhang

Recommended strategies:

All the important subjects identified above should be continued in line with individuals' expertise. At the same time, it would be good to further incorporate the methodology of (i) into existing research. Research in (ii), for example, is a field that has largely benefited from the approach of (i). Likewise for some parts of (iv).

At the same time, for the future developments of (ii), integration among researchers specializing in various aspects of the problem, namely, cryptanalysis, coding theory, statistical analysis, theoretical and experimental physics, would have to be carried out. It's only with this integration that we can hope to catch up with one of the few quantum technologies that have in fact been commercialized. At least, we should develop enough expertise within the community to evaluate whether a commercial quantum key distribution device indeed does what it claims to do or to be able to develop a product of this kind that would place us in a niche. Although there's already an ongoing effort to integrate the expertise among some of the theoretical teams and an experimental team for the actual implementation of quantum key distribution protocols, general interests in this area are still too limited.

Similarly, without a critical mass of people working in (b), our theoretical contributions to the ongoing competition in quantum computation would most likely be marginalized.

Although (iii) and (iv) involve some of the more controversial research topics in physics, they are at the same time, quite possibly the research areas where important breakthroughs are to be expected.

Recommendations on future hires:

New hires are strongly encouraged to work on (i), where there are still plenty of new things to attempt. On the other hand, new hires who are interested in the long-term development of quantum technologies should be encouraged to work on (ii). The more courageous newcomers, on the other hand, are welcome to attempt (iii) and (iv).

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TG2: High Energy Physics and Astrophysics

TG2.1: High energy phenomenology

The ultimate goal of studying cosmology and astrophysics is to answer such big questions as how the Universe starts, how it evolves to the current state, and how it will become in the future. To answer these questions and understand the underlying mechanisms, particle physics generally plays a very important role. In the early Universe when all substances exist in their fundamental forms (quarks, leptons, gauge bosons as we know today) at high temperatures and high densities, all dynamics are governed by the physical laws of elementary particles. The fundamental ingredients and their interactions thus determine what we observe about the Universe (relic density of dark matter, cosmic microwave background radiation spectrum, etc) now. Even today, the evolution of certain astronomical objects (e.g., supernovae, neutron stars, etc) still relies crucially on the dynamics of particles with most feeble interactions (e.g., neutrinos) with others.

The Standard Model (SM) of particle physics as we know has been a very successful model (perhaps qualified as a theory by now) in explaining countless particle reactions or processes in ground experiments and astronomical phenomena. (An excellent resource to find most up-to-date data and our theoretical understanding in various aspects is the document maintained by the Particle Data Group [2.1.1].) Even though all the elementary particles predicted in the SM have been confirmed in the laboratory and examined to have the properties decreed by the model, there are solid empirical facts and certain theoretical requirements that the SM cannot explain or satisfy. For example, we know the existence of cold dark matter (DM) through their gravitational effects at large scales, yet the SM does not possess a suitable candidate. We know neutrinos have mass from their oscillation phenomena, while it is not clear whether it has the same origin as the mass of other particles because their masses are found to be at least six orders of magnitude smaller than the electron.

Theoretically, it is difficult to understand why there is a large gap between the electroweak scale (≈O(100) GeV) and the Planck scale (GeV) if no new physics shows up in between (the hierarchy problem), and how to stabilize the Higgs boson mass at 125 GeV under radiative corrections (the naturalness). There is no good explanation why the masses of the charged fermions span almost six orders of magnitude, let alone the neutrino masses below eV, as well as their pattern (the flavor problem). It is also well-known that two of the Sakharov conditions (CP violation and out-of-equilibrium) are not met satisfactorily by the SM (the baryon asymmetry problem). Since the electroweak sector in the SM would result in merely a cross-over in the electroweak phase transition, it seems inevitable to extend the model in order to have a sufficiently strong first-order phase transition for baryogenesis.

Traditionally, particle physics phenomenology studies more phenomenological aspects of high-energy physics and plays the role of a bridge between pure high-energy theory and high-energy experiments. In view of the above-mentioned shortcomings of the SM, particle physics phenomenology has expanded its realm over the years to cover more aspects of the research of cosmology and astrophysics (e.g., phase transitions in the early Universe, gravitational waves, stellar cooling, etc). We consider the following more specific questions/topics to be of great importance and urgency:

1. Could the 125-GeV Higgs boson be a composite particle with new underlying dynamics? Are there more elementary particles and, if so, what is the connection between them and the SM particles (or even cosmology)?
2. What is the identity of DM? How does it interact with SM particles other than gravitationally?
3. What is the correct mass hierarchy or even their mass values? What is the mechanism for their mass generation? Are neutrinos Dirac or Majorana fermions? In the latter case, what are the CP-violating Majorana phases?
4. Besides the CP violation in the quark sector as depicted in the Kobayashi-Maskawa mechanism, are there new CP-violating sources to produce required matter-antimatter asymmetry of the Universe? How large is CP violation in the lepton sector?

5. How does strong dynamics work to produce the observed hadron spectrum? Why is there almost no CP violation in the strong sector?
6. Does Nature have more symmetries (e.g., gauged, supersymmetry, etc) and thus new particles within our collider reach? Are all the interactions unified under one simple framework?

Answering any of the above questions will definitely lead us to a new territory in particle physics. There are of course many other equally interesting mysteries and questions to be answered, yet we reckon that the above-mentioned are more likely to be tackled with existing theory tools and experimental facilities.

In Taiwan, we have constantly about 20–30 faculty members at various institutes, along with their research associates, focusing on research in particle physics phenomenology. On the other hand, we also have many high-energy experimental colleagues participating in different international experiments, such as ATLAS and CMS groups at the CERN LHC, Belle-II at KEK, Daya Bay, Juno, KOTO and TEXONO. We therefore hope that the two communities have close interactions (in the formats of discussions, joint meetings, etc) and, through such synergy, achieve breakthroughs at various fronts of research.

In the following, we detail the subfields in particle physics phenomenology. The topics are listed purely according to the alphabetical order. Such a topic division is largely for the convenience of presentation, and it is acknowledged that many of the discussed issues are inter-correlated.

(1) Cosmology and Astroparticle Physics

Cosmology and astroparticle physics have become important avenues at the interplay between particle physics and neighbouring fields. A huge amount of international efforts toward understanding the Universe, spanning from our solar system to the large scale structure, can be found in [2.1.2, 2.1.3]. For cosmology, important issues beyond the successful ΛCDM model include e.g., inflation, electroweak (EW) phase transition, matter-antimatter asymmetry, small scale challenges, the Hubble tension, and the detection of cosmic neutrino background (CνB). Finding answers to these issues can lead to breakthroughs in understanding fundamental physics at energy scales far beyond the reach of conventional laboratory experiments, as well as the nature of dark matter and dark energy. Different phenomenological particle physics models have been proposed as solutions to these questions and issues, which can possibly be tested by future observations; e.g., next generation cosmic microwave background missions (CMB stage-4, PICO, CORE, etc.) [2.1.4], ongoing and future gravitation wave (GW) experiments (LIGO-Virgo-KAGRA collaboration, eLISA, DECIGO, SKA, etc.), and the CνB experiment like PTOLEMY. For astroparticle physics, forefront issues include e.g., the origin of the extragalactic ultra high-energy cosmic-rays (CR), sources of high-energy astrophysical neutrinos, precise measurement of solar neutrinos, the detection of supernova neutrinos[1]. With future CR and neutrino detectors like CTA, GRAND, IceCube-Gen2, JUNO, DUNE, and Hyper-K, answers or important clues to these topics can potentially be delivered in the coming decades.

Talents in Taiwan: In Taiwan, nearly all these frontier topics are being actively pursued by researchers in different institutes, e.g., inflation and primordial black holes; EW phase transition and their GW signals; leptogenesis and baryogenesis; fuzzy dark matter and small scale problems; CνB detection; high-energy neutrinos; CR interactions; supernova neutrinos. Active theory members include: P. Chen (NTU), K. Cheung (NTHU), C.W. Chiang (NTU), T.H. Chiueh (NTU), H.T. Cho (TKU), Anatoli Fedynitch (AS), C.Q. Geng (NTHU), X.G. He (NTU), K.C. Lai (CGU), D.S. Lee (NDHU), W.L. Lee (NTNU), C.M. Lin (NCYUT), G.L. Lin (NYCU), K.W. Ng (ASIoP), H.Y. Schive (NTU), M. Spinrath (NTHU), Po-Yan Tseng (NTHU), M.R. Wu (ASIoP).

Looking forward over the next decade, we anticipate that missions mentioned above will bring vast amounts of observational data with much improved precision for all major directions in cosmology and

[1] We refer the discussions related to DM searches (e.g., anti-proton/helium, -ratio, GCE, CR-DM interaction, etc) to Sec. 3.

astroparticle physics. Synergetic efforts from both theory and observation sides of Taiwan's current and newly-hired cosmologists, astroparticle physicists, and astronomers can largely boost the impact and visibility of our teams on the international stage. In particular, potential addition of talents who work on e.g., precision cosmology modeling that can take into account a wide class of particle physics phenomenological models; the production, interaction, and propagation of high-energy cosmic-rays, neutrinos, and gamma-rays inside galaxies and astrophysical environments, can potentially bridge the

S strengths	• A strong computational group for wave DM (NTU) • Active recently in inflation and EW phase transitions (ASIoP & NTU) • Topics related to CCSNe and low-energy neutrinos (ASIoP, NTHU, NCTU)
W weaknesses	• Lacking experts in axion cosmology or neutrino cosmology • Lacking theory groups working on cosmic-ray transport • Lacking experienced modelers for high-energy particles
O opportunities	• Existing strong experimental groups including AMS (ASIoP) and ANITA(NTU) • Potential collaborations with newly-hired local astrophysicists • A couple new hirings (ASIoP & NTHU) boosting astroparticle physics
T threats	• Several strong competing groups in east Asia on cosmological GW signals

existing gaps between particle physics phenomenologists and observations to strengthen the synergy of the community and to harvest the upcoming astronomical and particle physics data.

(2) Dark matter physics

Observations from astronomy call for a non-luminous matter beyond the Standard Model, dubbed dark matter (DM). Several candidates for dark matter have been proposed in the literature: primordial black holes, a sterile neutrino that is a singlet under the SM, an axion that naturally solves the so-called strong CP problem in QCD, and weakly interacting massive particle (WIMP) [2.1.5]. Particle physicists in Taiwan mainly focus on the last two cases.

To declare the discovery and extract more information of dark matter, including its mass and spin, three search strategies are adopted: direct search, indirect search and collider search. Direct search experiments look for the signals of recoil energy of nucleus when DM hits the detector, which is typically at the order of keV.[2] The differential cross section of DM scattering off the atomic nucleus can have contributions from spin-independent (SI) and spin-dependent (SD) parts. Currently we have upper limits on the spin-independent and spin-dependent cross sections of dark matter with nucleon from XENON experiment, since no signal is observed. Indirect searches mainly aim at the cosmic rays produced by the dark matter within the Milky Way through either annihilations or decays into, e.g., neutrinos, gamma rays, positrons and antiprotons. For collider searches after the dark matter is produced at colliders, particularly the Large Hadron Collider (LHC), dark matter particles just escape the detectors and do not leave tracks. The

[2] However, if DM is lighter than about 1 GeV, the kinetic energy of recoiled nuclei would decrease significantly. The DM would rather scatter off the electron in this case. Correspondingly, signals of DM scattering off electrons offer better probes than DM–nucleon scattering.

searching strategy is to look for the missing energy in company with visible SM particles, for example jets, leptons or photons. Therefore, the signals would be model-dependent.

Talents in Taiwan: Surely, dark matter is one of the main focuses of theoretical particle physics, and a wide range of topics are covered by research groups in Taiwan, including Academia Sinica (K.W. Ng, M.R. Wu, T.C. Yuan), NTU (J.W. Chen, C.W. Chiang, X.G. He), NTNU (C.R. Chen, F.L. Lin), Tamkang University (C.S. Chen), CYCU (K.C. Yang, C.K. Chua), NTHU (W.F. Chang, K. Cheung, C.Q. Geng, M. Spinrath, Po-Yan Tseng), NYCU (G.L. Lin), NCKU (C.H. Chen) and NDHU (C.P. Liu, H.C. Chi). Studies done include: Model building focuses on proposals of concrete models that aim to solve one or more experimental anomalies; cosmic-ray positron excesses; constraints from cosmic gamma-ray, antiproton and neutrino, sub-GeV dark matter; and self-interacting dark matter. In particular, after searching for O(10-100) GeV WIMPs for many years, light to ultra-light dark matter scenarios receive a lot of attention in recent years [2.1.6]. Dark matter may have an influence on astrophysical observations as well [2.1.7]. Topics include formation of hybrid stars and neutron stars, and its impacts on gravitational wave signals; structure formation; 21-cm absorption spectrum observed by EDGES; and core-collapse supernovae. Also, the interplay between dark matter and various topics have also been studied, covering early universe, neutrino, colliders and muon physics.

All these clearly illustrate the versatile contributions from different groups in Taiwan on DM-related researches. Keeping this momentum going while exploring new opportunities with novel experimental techniques or astrophysical probes will be the major directions in the next ten years. To achieve this, dedicated cultivation to the next-generation physicists including students and postdocs working in this direction is highly desired. A SWOT analysis is given below.

S strengths	• Dark Matter theoretical modeling • Established in global analysis for WIMP searches. • Interplay between theoretical scattering calculations and experimental germanium/xenon detections. (AAS, NTU, NDHU) • Dark Matter Signals on Collider Physics.
W weaknesses	• No large-scale on-site experimental collaborations. • Lacking young theorists participating in major international experiments.
O opportunitie s	• Interplay between theoretical studies and experimental detections. • Probing the DM origins with astrophysical multi-messages signals (Gravitational Waves, neutrinos, and multi-wavelength EM waves). • New experimental set-ups (proposals) for non-WIMP DM candidates
T threats	• Cultivate young generations.

(3) Flavor physics

The SM has been well tested by precision measurements in high energy experiments. However, it is taken as an effective theory at the electroweak scale because of such unsolved problems as origin of neutrino mass, matter-antimatter asymmetry, and dark matter. The potential topics in flavor physics that we are studying and will investigate are briefly summarized below.

Top quark flavor-changing neutral currents (FCNCs) are extremely suppressed in the SM due to the Glashow-Iliopoulos-Maiani mechanism. The branching ratios for top FCNC processes in the SM are highly suppressed and are far below the detection limits of the LHC. The expected sensitivity in the high luminosity (HL) LHC with an integrated luminosity of 3 ab^{-1} at $\sqrt{s}$ = 14 TeV is in the range of $10^{-5} - 10^{-4}$. Thus, the top quark flavor-changing processes can serve as good candidates for investigating new physics effects. A promising hint for new physics is found in the muon g − 2 since the experiment at Brookhaven National Lab reported a 3.3σ deviation from the SM prediction. The new measurements performed at Fermilab (J-PARC) aim for a precision of 0.14 (0.10) ppm. It has now become an exciting research topic after Fermilab confirms the anomaly recently. Applying the accurate measurements of the fine structure constant to the theoretical calculations, it is recently found that the differences in the electron g − 2 between the experiment and the SM result are −2.4σ deviation [2.1.8]. Thus, the lepton sector now plays an important role in exploring new physics.

A proposal to search for the trace of new physics is the rare K-meson decays, where $K^+ \to \pi^+\nu\nu$ and $K_L \to \pi^0\nu\nu$ are theoretically clean. Both processes become attractive because the NA62 experiment at CERN is intended to measure $K^+ \to \pi^+\nu\nu$ with a 10% precision, and the KOTO experiment at J-PARC will observe $K_L \to \pi^0\nu\nu$. In addition, KLEVER at CERN could observe $K_L \to \pi^0\nu\nu$ at the precision of 20%. Recently, NA62 reported its first result using the data taken in 2016 and found one candidate event of $K^+ \to \pi^+\nu\nu$. It is time to further study these rare *K* decays. Several interesting excesses in semileptonic *B* decays have been reported by experiments. They are (i) angular observable P'_5 of $B \to K^*\mu^+\mu^-$, (ii) the ratios $R(D^{(*)})$, and (iii) the ratios $R(K^{(*)})$. LHCb reported P'_5 with a 3.7σ deviation from the SM prediction since 2013, and the updated result in 2020 still shows the deviation. The measured $R(D^{(*)})$ and $R(K^{(*)})$ show the significant deviations from the SM predictions. They are important because the SM predictions have small theoretical uncertainties. It is believed that the *B*-anomalies will continue to be a hot topic in the near future [2.1.9].

In the next few years, we will devote ourselves to the relevant studies and find interesting connections to other phenomena, such as neutrino physics, dark matter, and collider physics. We also look forward to more precision data coming from Belle-II, BESIII, LHCb and even the HL-LHC and HE-LHC in the farther future [2.1.10].

S strengths	• K_T resummation in PQCD theory (ASIoP), generalized QCD factorization (ASIoP, CYCU, NTU), and SU(3) flavor symmetry (NTU) for nonleptonic B/D decays in the SM • Familiar with various SM extensions in B, D, and K meson systems and in lepton sector (NTU, NTHU, NCKU)
W weaknesses	• Few young graduate students involved • Less comprehensive analysis in UV-complete theories • Less experience in full RG running in new physics model
O opportunities	• Learning the latest progress in rare B decays from Belle II (NTU) more directly • Learning the potentially exotic events in rare K decays at J-PARC KOTO group (ASIoP, NTU)
T threats	• Soft-Collinear Effective Theory approach in B physics in USA and European groups • Potentially competing groups in BSM flavor physics from around the world, such as KEK, Nagoya U., KIAS, and groups in India, USA, and Europe

Talents in Taiwan: Here we list active theorists working on various issues in flavor physics in Taiwan: C.H. Chen (NCKU), H.Y. Cheng and H.n. Li (ASIoP), C.W. Chiang, X.G. He, T.W. Chiu and W.S. Hou (NTU), C.K. Chua and K.C. Yang (CYCU), and C.Q. Geng (NTHU). In the heavy flavor physics, we have people working on different approaches: QCD factorization and perturbative QCD in a perturbative fashion, and lattice QCD and flavor SU(3) symmetry in a non-perturbative fashion, offering sufficient diversity for comparison just within Taiwan. We would like to mention that close interactions between these theorists and our experimental colleagues working on the Belle experiment at KEK had produced a great success in the 2000s and led to a win-win situation for both experimentalists and theorists. This scenario is what we are looking forward to in the coming years for all subfields. A SWOT analysis is given below.

(4) Higgs physics

The SM of particle physics has been completed after the discovery of the 125-GeV Higgs boson in the summer of 2012. Even though its many properties are found to be consistent with SM expectations within uncertainties, it is nevertheless a pressing task to determine its couplings with other particles with high precision, in anticipation of possible footprints of new physics. The Report of the Particle Physics Project Prioritization Panel (P5) lists "Use the Higgs boson as a new tool for discovery" as the first scientific opportunity [2.1.11]. Because of the uniqueness and special role of the Higgs boson in particle physics, it is highly advocated that we should push for building a Higgs factory based upon an electron-positron collider of suitable energy [2.1.12].

We have been constraining the Higgs-boson couplings with the available data from the LHC experiments, and constantly updating the results whenever the dataset received substantial improvement [2.1.13]. In some analysis, we observe a trend that the overall Higgs strength shows a 2σ surplus that is worth close monitoring when the LHC restarts again. Any deviations in the Higgs couplings would hint at extensions in the Higgs sector. For example, we have studied the general two Higgs doublet model (g2HDM, used to be called 2HDM-III). In a series of analyses, the second diagonal top Yukawa is found to be naturally $O(1)$ and complex, which is capable of driving electroweak baryogenesis and accommodating the electron EDM bound by ACME 2018. Being very well motivated, the model has a potentially rich search program at LHC, which overlaps well with the Belle II and CMS flavor program in Taiwan. We have also studied the Georgi-Machacek model, which features the existence of a doubly charged Higgs boson and other interesting phenomena. We have done quite a few pioneering phenomenological studies on the model, including the calculations of full one-loop renormalized Higgs couplings for future comparison with precision Higgs coupling measurements at HL-LHC and CEPC/ILC. There are also many other phenomenological studies in the usual 2HDM, gauged 2HDM (G2HDM), Higgs-portal models, supersymmetric models. It is worth mentioning that there is also a significant effort in studying composite Higgs models and Higgs-Yukawa models using, due to the underlying non-perturbative strong dynamics, lattice simulations that involve big international collaborations.

Vector boson scattering (VBS) forms an important class of processes for probing the electroweak symmetry breaking (EWSB) within and beyond the SM. The CMS group is involved in the HGCal upgrade of the endcap detectors in Phase II for detecting forward jets in VBS events. We have been doing detailed collider simulations, including the utilization of deep machine learning techniques to improve the efficiency in jet charge determination, reducing ambiguity in events with missing energy, distinguishing different production mechanisms of Higgs boson, etc. Finally, another intriguing direction is the existence of a hidden sector that communicates with the SM sector weakly. A peculiar signature in this class of models is the existence of long-lived particles (LLPs), whose experimental detection would involve new technologies and challenges. We have performed some model studies about how to detect the LLPs at colliders.

Talents in Taiwan: In summary, the above-mentioned studies of Higgs physics at the LHC have put Taiwan at a relatively advantageous status. Theorists currently active in this direction include: C.H. Chen (NCKU), C.R. Chen (NTNU), C.S. Chen (TKU), K. Cheung and Po-Yan Tseng (NTHU), C.W. Chiang and W.S. Hou (NTU), and T.C. Yuan (ASIoP). The following is a SWOT analysis for the subfield of Higgs physics in Taiwan.

S strengths	• Having established grounds in g2HDM (i.e., 2HDM-III), GM, HTM, and related Higgs models • Having some experience in comprehensive/global analysis
W weaknesses	• Lacking people actively working on loop corrections • Lacking own codes for numerical analyses • Lacking junior faculty members (in their 30s) on this topic
O opportunities	• Having NTU CMS group focusing on g2HDM • Using machine learning techniques as a new approach to help studying Higgs physics
T threats	• A big group in Japan (led by Osaka) expert in and having a code for Higgs couplings of simple BSM Higgs models at one loop

(5) Neutrino physics

Neutrinos have played many important roles in particle physics since they were postulated. Nevertheless, to this day there are still many open questions about neutrino properties, for instance, if they are their own antiparticles or not, their origin of mass, CP violation, etc. Furthermore, in recent decades they played an increasingly important role in astroparticle physics where they are one prong of the multimessenger program complimentary to photons and gravitational waves with some unique advantages, see also Section (2) above on dark matter physics. For a recent review on opportunities at next-generation neutrino experiments see [2.1.14], a review on high-energy astrophysical neutrinos see [2.1.15], and for a white paper on neutrino theory [2.1.16].

In Taiwan several groups have worked on various aspects of neutrino physics, from some early seesaw models speculating about their origin of mass, over connections to Grand Unified Theories, searches for heavy neutrinos at colliders to questions closely related to ongoing and upcoming neutrino experiments like Super-Kamiokande and JUNO.

In particular, Taiwan has gained some outstanding international reputation for model building and properties of low energy neutrinos. With the retirements of X.G. He (NTU) and C.Q. Geng (NTHU) there has emerged an urgent need to hire new young faculties to fill the gap and keep neutrino physics in Taiwan alive. At the time of writing it seems advised to focus on researchers, who work on the interplay of particle physics, astrophysics and cosmology, where neutrinos play an extremely important role as mentioned already.

Talents in Taiwan: PIs in Taiwan, who have worked or are working on theoretical aspects of neutrino physics in recent years (in alphabetical order): W.F. Chang (NTHU) C.H. Chang (NTNU), C.H. Chen (NCKU), K. Cheung (NTHU), C.W. Chiang (NTU), S.H. Chiu (CGU), Anatoli Fedynitch (AS), C.Q. Geng (NTHU), X.G. He (NTU), G.L. Lin (NYCU), M. Spinrath (NTHU), and T.C. Yuan (AS).

S strengths	• Outstanding international reputation • Particularly strong in model building • With TEXONO some of the best results in low energy neutrino physics
W weaknesses	• Comparatively weak in neutrino cosmology, one of the important fields in the future • Lack of coherent efforts, i.e. many small groups working on different aspects who merely interact
O opportunities	• With the ANITA group at LeCosPa and the JUNO group at NTU and NYCU potential collaborations with experimentalists
T threats	• Japan has a long-standing tradition in theoretical neutrino physics • With Hyper-K in Japan, JUNO in China, RENO in South Korea, etc. other countries in the region have strong experimental commitments

(6) Neutrinos in Nuclear Physics

Nuclear physics has been and will keep playing an indispensable part in our continuing quest of neutrino properties and their role in astrophysics and cosmology. In the next decade, the KATRIN experiment will have the best mass measurement of the electron neutrino [2.1.17]; several flagship oscillation experiments: DUNE, Hyper-Kamiokande, and JUNO will provide more precise determination of neutrino mixing parameters [2.1.18], including the possible CP-violation phase; and experiments to look for neutrinoless double beta decay will shine a light on the Dirac or Majorana particle nature of neutrinos [2.1.19]. In the meantime, these sensitive neutrino detectors, either stand-alone or multipurpose for dark matter and gravitational waves, are able to see the neutrinos from the Sun, supernovae, and other interesting astronomical sources. They will reveal some of the inner mysteries of these objects and the Cosmos.

Talents in Taiwan: Currently in Taiwan, J.-W. Chen (NTU), H.-C. Chi (NDHU), and C.-P. Liu (NDHU) are working on topics involving neutrino-atom and elastic neutrino-nucleus scattering. Together with the TEXONO Collaboration (ASIoP), their series of works on the neutrino magnetic moments and millicharges fully demonstrates the importance of many-body physics and their cross-section calculations among the best in literature. M.-R. Wu (ASIoP) and his collaborators are working on topics involving neutrinos in hot-and-dense stellar environments including supernovae and neutron star mergers. Their works contribute to the understanding of collective neutrino flavor conversions, heavy-element nucleosynthesis, and neutrino-nuclear matter interactions.

In the next decade, we expect the frontier neutrino research programs in both experiment and astronomical observation will still heavily rely on nuclear theory inputs. Our attention will be on the relevant electroweak processes such as nuclear beta decay and neutrino-nucleus reactions, either in vacuum or media. Therefore, we think it is timely to develop our local expertise on nuclear many-body physics in nuclei and nuclear matter, and recommend NCTS taking this area into account upon hiring.

(7) Strong Interaction Physics

Quantum Chromodynamics (QCD) is an important part of the standard model which describes the interaction among quarks and gluons in quantum field theory. This theory is perturbative in high energies, which makes the analysis in principle easier, but becomes non-perturbative at low energies, which makes it challenging to solve. Many problems in particle physics have their largest uncertainty from strong interactions and hence many breakthroughs are directly related to advances in the treatment of strong interaction physics. For example, at low energies, the development of various effective field theories (EFT's) of QCD to use different expansion parameters other than the coupling constant has led to tremendous progress of particle and nuclear physics in the past. Also, the development of lattice QCD, which puts QCD on a spacetime lattice and performs the direct numerical computation of QCD, has become an indispensable tool to particle physics. (See the QCD review in [2.1.1].)

Talents in Taiwan: The QCD community in Taiwan is small but well known in perturbative QCD (Hsiang-nan Li (AS)), EFT(Jiunn-Wei Chen (NTU)), lattice QCD (Ting-Wai Chiu, Jiunn-Wei Chen (NTU)), and quark-gluon plasma (Di-Lun Yang (AS)). In the next decade, our expertise and common interests overlap nicely with those of the next generation experiments of electron ion collider (EIC) which will be built in Brookhaven National Laboratory (BNL) [2.1.20] and perhaps also in China (EicC) and CERN (LHeC). This common theme of study between theory and experiments is how properties of hadrons and nuclei are formed by quarks and gluons. In particular, the primary goals of EIC are to study the gluon distributions and three-dimensional parton distributions in hadrons and nuclei. Recent breakthroughs of lattice QCD and early numerical studies and later state-of-the-art calculations (JW Chen) both have shown great promise on direct computations of those quantities on the lattice (see [2.1.21-22] for recent reviews). However, more studies such as the factorization theorem (HN Li) and perhaps the use of lattice chiral fermions (TW Chiu) will be critical. And whether the method can be extended to the study of fragmentation functions, which are crucial in exclusive and semi-inclusive processes, is of great interest. How quark current responses to an external magnetic field or vortex flow (DL Yang) will remain an important issue of study as well.

(8) Other Interesting Topics and Important Issues

In the following, we list a couple more topics that are thought to be of sufficient importance or interest and, therefore, the community in Taiwan should consider in their future faculty hires:

(1) In view of the axion search experiment (under the joint efforts of National Central University, National Chung Hsing University, National Synchrotron Radiation Research Center, and the Institute of Physics at Academia Sinica), we think it should be better to have at least one axion expert as theory backup.
(2) Taiwan is a strong collaborator in the gravitational wave detectors LIGO and KAGRA. On the theory side though, there are some weaknesses. In particular, we would recommend hiring an expert working at the interplay between particle physics and cosmology. In this field we expect major breakthroughs in the next decade.

High energy phenomenology in Taiwan has a serious age issue. In the past 10 years or so, the entire community has only hired five faculty members (Chian-Shu Chen, Chuan-Ren Chen, Martin Spinrath, Meng-Ru Wu, and Di-Lun Yang) while in the same time six retired (Pisin Chen, Hai-Yang Cheng, Chi-Yi Cheung, Ting-Wai Chiu, Chiao-Qiang Geng, Xiao-Gang He). Many more will likely retire within the next ten years. To keep the field alive and benefit from the reputation Taiwan has gained in the last decades, there is an urgent need for the community to hire more active, young faculty members.

NCTS can play a key role for the above purpose. We plan to hire talented postdocs who show great potential to become future faculty members in Taiwan. During their time at NCTS we will actively promote them if they perform well and demonstrate themselves in front of the community as potential faculty candidates. This might in particular help also to attract foreign talents who might otherwise not be considered in hiring processes.

NCTS is also pursuing the strategic goal of substantially increasing gender balance and diversity of its members and with equal qualifications we will prefer minorities when hiring. This TG of NCTS will make efforts to support various international meetings/schools, including those existing and future joint international activities, to be hosted at different institutes in Taiwan.

(9) Summary

We summarize this document by providing the following SWOT analysis for the theoretical high-energy and medium-energy physics communities in Taiwan:

S strengths	• We have already built up international reputation on various topics • We have many students with talent, enthusiasm, and creativity • Many of our colleagues remain active in research even when they are retired or close to retire • Given common interest, it is relatively easy for people to meet and collaborate
W weaknesses	• Being a small country, Taiwan has difficulty in forming sizeable groups on the research of many important topics • We are in desperate need for more active young blood to inject new ideas as well as continue our legacy • Our salary system and research funds are generally less attractive • Talented students prefer to pursue PhD abroad
O opportunities	• NCTS may offer a good platform to bring researchers at different institutes together to produce some works that are otherwise impossible • NCTS may organize for students intense courses on frontier topics that are otherwise impossible/impractical at individual institutes • We can work closely with China or Japan if any new collider is built in these countries
T threats	• As a neighboring country with same language and similar life culture, China is rising fast and strong and offers many good opportunities for young people, with great salaries and research resources that could compete with advanced western countries • China or Japan could take the lead in particle physics if they build the next colliders.

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TG2.2: High energy theory

Important directions in the next decade:

(1) Confluence of advancement in cosmology, conformal field theory correlators, and flat-space S-matrix:

Constraining the space of consistent theories can be cast into delineating the boundaries of consistency for physical observables. Such a model independent approach to physics has taken root in vastly distinct fields with distinct focuses. This includes the bootstrap program in conformal field theories (CFT), giving predictions on spectrum and couplings in any consistent CFT [2.2.1], as well as novel analytic understandings of scattering amplitudes in QFT [2.2.2], and more recently in cosmological correlators [2.2.3]. Since these approaches share a common philosophy, it is clear that their techniques and implications can be introduced across fields. Via AdS/CFT, the correlation functions that are subject to bootstrap methods can be related to flat space S-matrix in the infinite AdS radius limit [2.2.4]. This implies a new bootstrap approach to constructing amplitudes for consistent UV complete theories. In turn, the knowledge of the flat space amplitude also imposes new constraints on the boundary CFT correlator. On the other hand, flat-space S-matrix controls the non-analyticity of cosmological correlators. This connection has only recently begun to be explored and led to results that were not attainable from traditional methods. Such confluence of fields has been selected as one of the major funding topics by the Simons Foundation.

(2) AdS/CFT, Quantum information and fundamental physics

The Ryu and Takayanagai formula for the entanglement entropy of a quantum system [2.2.5] with its environment has led to various important advances in our understanding of gravity and the quantum nature of spacetime. The duality relation has also allowed one to formulate and study problems of quantum information theory in terms of geometric quantities in the bulk. As realistic quantum devices are always of finite extent, the formulation of holographic principle is even more interesting and relevant for QFT with boundary. Since the proposal of Takayanagai for boundary holography [2.2.6], a number of novel results have been uncovered for boundary QFT, including the discovery of a number of novel fundamental effects [2.2.7] in QFT that can be measured. Boundary holography not only provides a powerful formalism to tackle non-trivial boundary phenomena, it can also be expected to have an impact on the more practical side such as the design and manipulation of quantum devices and quantum control. The increasing interactions among quantum information, theoretical computing, and high energy physics communities will almost certainly bear fruits in the coming decade.

(3) Amplitude and gravitational waves

The connection between scattering amplitudes of point-like particles and the conservative potential of inspiral gravitational objects, have for the past few years brought tremendous progress in the Post-Newtonian expansion of gravitational observables, which feeds into precision computations of waveforms for gravitational waves generated by inspiral objects. We anticipate the continued progress will not only lead to a breakthrough in precision GR predictions, but more importantly a deeper understanding of the long range observables of black holes, such as the underlying principle for vanishing black hole Tidal Love number and the imprint of black hole horizons on gravitational wave signals.

(4) Machine as a high energy theorist

Theoretical high energy physics often follows the top-down, UV to IR approach in constructing the suitable models, which yield definite predictions to compare with the experimental data. This approach can however be susceptible to become biased towards certain aesthetically pleasing models. With the expected large amounts of data from the upcoming astronomical, gravitational and high energy experiments, these serve as the ideal training data for the machine-learning (see e.g. [2.2.8]). The hope is that with sufficient training, the machine will directly reconstruct the suitable class of models capturing the underlying physics, without prior biases, furthermore making concrete predictions for experimental verifications. This direction will partially replace the traditional top-down model building approach in astronomy and high energy theory, when tackling the experimental data.

Talents in Taiwan:

Since the mid nineties, the hep-th/gr-qc community in Taiwan has enjoyed a steady growth, beginning with Jen-Chi Lee (NYCU), Pei-Ming Ho (NTU), Chong-Sun Chu (NTHU), Feng-Li Lin (NTNU), Chiang-Mei Chen (NCU), Chuan-Tsung Chan (THU), Yi-Yang (NYCU), Wen-Yu Wen (CYCU), Chen-Pin Yeh (NDHU), Heng-Yu Chen (NTU) and Yu-tin Huang (NTU) and Yi-Zen Chu (NCU), Dimitrios Giataganas (NSYSU). Many have made important contributions related to the topics mentioned above:

Application of machine learning in hep-th/gr-qc: Heng-Yu Chen, Dimitrios Giataganas, Feng-Li Lin.
The holographic correspondence and its applications: Chiang-Mei Chen, Chong-Sun Chu, Dimitrios Giataganas, Pei-Ming Ho, Wen-Yu Wen, Chen-Pin Yeh.
Theoretical understanding of black holes: Chiang-Mei Chen, Chong-Sun Chu , Pei-Ming Ho, Wen-Yu Wen.
Scattering amplitudes and CFT correlators: Heng-Yu Chen, Yu-tin Huang, Jen-Chi Lee, Yi Yang,
Gravitational waves: Chong-Sun Chu, Yi-Zen Chu, Yu-tin Huang, Feng-Li Lin.

Recommended strategy and Teams to watch:

On the specific research directions mentioned previously, Taiwan's local resources and collaborations are also well positioned to make an important impact.

(1) Cosmological Bootstrap:

In the confluence of CFT/Cosmological correlators and flat space scattering amplitudes, Heng-Yu Chen (NTU) and Yu-tin Huang (NTU) are working actively on CFT correlators and scattering amplitudes respectively. Furthermore, Daniel Baumann (Amsterdam Univ), a renowned young researcher in theoretical cosmology who is one of the leading founders of the cosmological bootstrap program, has frequently visited Taiwan for long durations and will soon take on a three-year Jade Mountain Young scholar appointment. This with our existing international collaborations, including young researchers such as Prof. Tatsuma Nishioka (Tokyo Univ), Prof. Toshifumi Noumi (Kobe Univ) and Prof. Sangmin Lee (Seoul Nat. Univ), we are in a very unique position to make a strong footprint in this upcoming field.

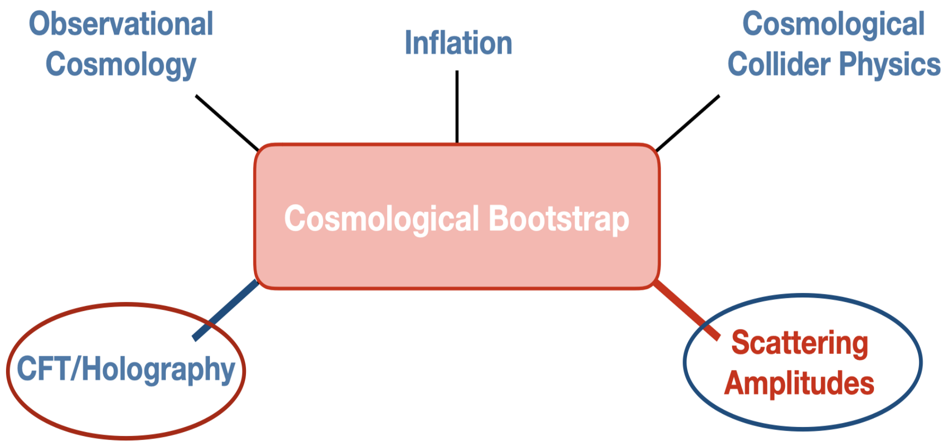

FIG.2: Heng-Yu Chen, Yu-tin Huang (NTU) and Daniel Baumann (Amsterdam Univ), together with other existing international collaborators, are in a very unique position to make a strong footprint in this upcoming field of Cosmological Bootstrap.

(2) Black Hole Initiative:

There are also a number of local faculties in Taiwan that are now actively working on various aspects of black hole dynamics, Chiang-Mei Chen (NCU), Pei-Ming Ho, Yu-tin Huang (NTU), Chong-Sun Chu (NTHU), Feng-Li Lin (NTNU), Yi-Zen Chu (NCU), with various degrees of connection to the observables in gravitational wave signatures, including the nature of black hole horizons, memory effect, Hawking radiation, quasinormal modes, and Tidal love numbers for black holes and neutron stars. Moreover, there are also several young Taiwanese researchers that are currently in leading research groups in these areas such as Chia-Hsien Shen (UCLA) and Wei-Ming Chen (Amsterdam Univ) that are in leading research groups in these areas. Importantly, we have researchers working in or associated with Taiwan that populate the three pillars of the modern approach to precision waveforms as shown in the diagram below. NCTS can serve as a platform to set-up a BLACK HOLE INITIATIVE. With joint web-seminars and events focusing on this topic, and further promoting interaction between the observation and theoretical side.

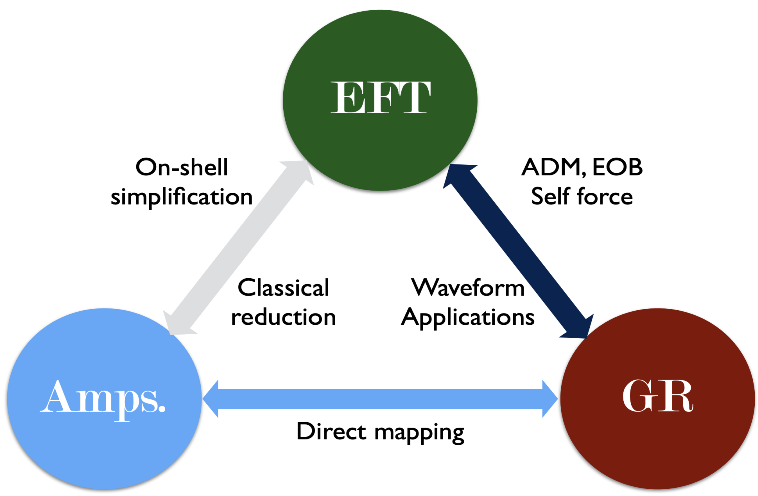

FIG. 3: BLACK HOLE INITIATIVE---We have researchers working in or associated with Taiwan that populate the three pillars of the modern approach to precision waveforms of black hole detection. NCTS can serve as a platform to set-up this initiative.

Research Teams to watch:

Recently, there is a growing list of names of more senior people who are scientifically active and have spent extended periods in Taiwan via visiting professorships, workshop organizers or short course lectureships, etc., such as Gary Shiu (UW-Madison), Daniel Baumann, Miranda Cheng (Amsterdam), Hikaru Kawai (Kyoto), to name a few. NCTS can provide these faculties with distinguished visiting professorship, with additional funding to support the running of short term programs, hosting of their individual research groups.

There are currently many excellent Taiwanese young high energy theorists working in the various areas, such as non-perturbative aspects of quantum field theories, scattering amplitudes, interface of condensed matter and high energy physics and conformal bootstrap program. Starting from Shu-Heng Shao who recently accepted a junior faculty position at Stony Brook University; Chi-Ming Chang who is a junior faculty in Beijing Tsinghua University; Po-Shen Hsin who is a highly creative postdoc at Caltech; Ying-Hsuan Lin and Juven Wang, who are both very productive senior postdocs at Harvard University; Chia-Hsien Shen, who is a successful senior postdoc at UCSD; Kuo-Wei Huang, who is a very independent postdoc at Boston University, to name a prominent few. In any research team building activities, it will be crucial to also take into account the potential contributions of these exciting young Taiwanese talents into the considerations.

Recommended Research Areas and Faculty Hiring Candidates:

(1) Non-perturbative investigations of quantum field theories, and their applications to cosmology, quantum information and condensed matter systems.

Over the past years, there have been rapid research developments in applying bootstrap techniques to impose powerful constraints on the physical data, such as the scaling dimensions, OPE coefficients, and particle spectra of various quantum field theories in different dimensions. These results enable us to carve out the physically allowed regions in the vast space of possible quantum field theories [2.2.9]. Often these distinct regions can be connected via different non-perturbative dualities, which have been actively investigated previously in supersymmetric and more recently non-supersymmetric settings, with the holographic duality being the prime example. It is highly desirable to apply these non-perturbative methods to constrain the incoming cosmological data, to probe novel effects in quantum information systems, and to uncover exotic phases in novel condensed matter systems. Local faculties such as Heng-Yu Chen, Chong-Sun Chu, Dimitrios Giataganas, Yu-Tin Huang along with postdocs and students have been heavily involved in these activities. NCTS will serve as an excellent collaboration platform for identifying the exciting topics and making concerted efforts to solve them. We would like to recommend universities and research institutions in Taiwan to hire junior faculties with research overlap in this area to reinforce the on-going research efforts.

(2) Applications of perturbative quantum field theoretic methods to decipher gravitational wave observational data and to make definite future predictions.

With the groundbreaking discoveries of LIGO/VIRGO collaboration [2.2.10], we have now firmly entered the era of gravitational wave astronomy. New interferometer observatories are expected to be operating in the coming decades, and with the deluge of new data, we expect to investigate gravity under extreme conditions with unprecedented precision. These developments have also spurred new research activities on the theory front, in addition to the traditional numerical relativity simulations of different events for the experimental comparisons. More recently, newly developed computational techniques for perturbative scattering amplitudes have been applied to compute higher order post-Minkowskian evolution, tidal effects and multi-body potentials, of compact gravitational objects. These results potentially lead to very exciting predictions for comparing with the future observational data. Local faculties such as Feng-Li Lin, Yi-Zen Chu, Yu-tin Huang along with postdocs and students have been heavily involved in these activities. We would also like to recommend junior faculty hirings with the research expertise in this area, along with numerical relativity and multi-messenger astronomy, as the potential collaborations among them will definitely put Taiwanese gravitational wave research on the world stage.

Additional recommendations:

Besides highlighting the specific targeted research areas and individual researchers for hiring, we would also like to make few general recommendations which NCTS can further support the current and the incoming theoretical physics faculties in Taiwan:

(1) Making joint offers of faculty/research positions to the exceptional candidate such that they can have a semester of research leave at NCTS annually (Similar arrangement exists for the faculties at YITP, Stony Brook.).
(2) Teaching reductions for the center scientists from their universities to help them to conduct cutting-edge research and make greater contributions serving the community.
(3) Providing the funding for temporary teaching buy-out to make key personnels available to organize long term workshops in NCTS (like in KITP).

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TG2.3: Theoretical and Computational Astrophysics

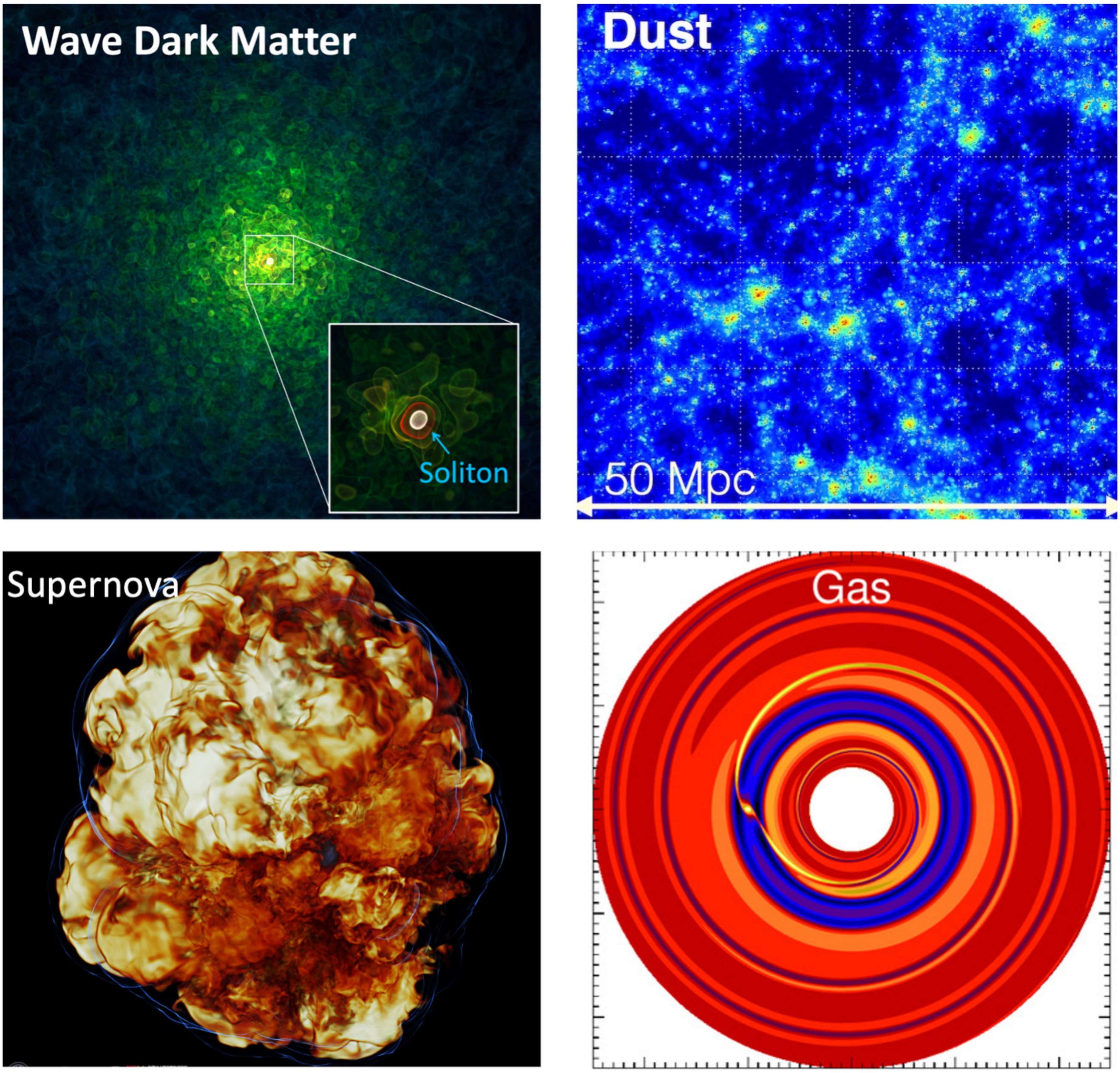

Figure 4: *State-of-the-art simulations of astrophysical phenomena in the four key research topics discussed in the text. These simulations were created by members of the NCTS-TCA group using mostly local HPC infrastructure, including the Taiwania-3 cluster at NCHC, the CICA cluster at NTHU, the Eureka GPU cluster at NTU, and the TIARA cluster at ASIAA. Top left: a wave dark matter halo (topic 1); top right: the distribution of dust in the cosmic web (topic 2); bottom left: a supernova explosion (topic 3); bottom right: a young protoplanet in a protoplanetary disk (topic 4).*

Important directions in the next decade:

We recommend four scientific and one technological field of focus for the Taiwanese theoretical astrophysics community in the next 10 years. Examples of the scientific topics are shown in Figure 4. Our recommendations are based on the original proposal to establish the Theoretical and Computational Astrophysics (TCA) Thematic Group at NCTS, which set out key topics for future development based on existing expertise at Taiwanese institutions. This white paper expands that vision to the next decade to bring Taiwanese astronomy to a world-leading status.

Taiwan is a major participant in several key international telescopes, for example ALMA (e.g. ASIAA) and KAGRA (e.g. NTHU). It is therefore necessary to support growth of the theoretical astrophysics community around the opportunities for science and collaboration provided by observations with these facilities. For example, NTU is leading the development of the advanced magneto-hydrodynamical code GAMER optimized for the use of high performance Graphics Processing Units (GPUs). However, such code-development efforts are not yet widespread in Taiwan and should be further promoted. In addition, although NCHC follows a successful model for centralized High Performance Computing (HPC) and is essential to our community, the wider HPC ecosystem in Taiwan is lacking two key ingredients for effective competition at an international level: institutional-level funding for mid-scale HPC and a framework for recruiting skilled technical support personnel. The table below presents a more complete SWOT analysis of Taiwnese theoretical astrophysics.

Strengths	● Many junior faculty hires in recent years in all of the identified key science areas, with strong track records in leading international centers and the ambition and expertise to develop the reputation of the community; ● Regular upgrades to computing hardware through the National Center for High-performance Computing (NCHC) with ongoing support for large-scale HPC; ● Participation of Taiwanese theorists in ongoing international astronomical collaborations;
Weaknesses	● Critical lack of support for technical staff to enable mid-scale HPC at the institutional level, reducing productivity and limiting training for junior researchers in comparison to international peers; ● Limited expertise in simulation code development; ●Difficulty in attracting top PhD students from overseas and poor support for postdoctoral researchers (salaries, benefits, esteem, career opportunities);
Opportunities	● Synergy between the development of an institute-scale HPCecosystem to support astrophysical research and the further development of NCHC; ● Investment from and collaborations with industry; ● Cost-effectiveness of a strong computational theory community in building Taiwan's international profile, with relatively low capital investment. ● The increasing worldwide emphasis on scientific HPC, both in astrophysical theory and the analysis of extremely large or novel astronomical datasets (some of which Taiwan is directly involved in developing).
Threats	● More visible established groups in Europe, North America, and Japan compete for the most productive postdoctoral talent; rapidly growing institutions in the region (e.g. in China and Korea) compete for recognition and influence in large collaborations.

(1) Dark Matter and Cosmology

Dark matter (DM) comprises ~85% of the matter in the universe. The existence of DM is confirmed mainly through its gravitational influence on the large-scale structure of the universe, individual and clustering of galaxies, and cosmic microwave background (CMB). However, despite decades of searching, DM still escapes from direct detection in particle colliders and underground experiments. As a result, the nature of DM remains largely unknown. For example, what are the DM particle mass and temperature? Is it collisional or collisionless? Does it have non-gravitational interaction with other matter and what is the corresponding cross-section? Will DM decay? How to distinguish the effects of DM from those of modified gravity?

Upcoming large telescopes such as JWST (2021), Euclid (2022), and WFIRST (2025) will soon transform our understanding of the universe and DM by probing, for instance, the formation and distribution of first stars and galaxies, the DM substructures in galaxies and galaxy clusters, and the faint-end slope of the luminosity function. In addition, next-generation surveys of high-resolution CMB polarization will put stringent constraints on the DM-photon and DM-baryon scattering cross-sections. It is thus timely and crucial for the theoretical and computational astrophysics community in Taiwan to strengthen collaborations for interpreting data and making observational predictions.

One important breakthrough in DM research from Taiwan is the field of alternative DM models, especially the study of wave/fuzzy dark matter (FDM) led by the NTU team (Figure 4, top left) This model has become increasingly popular because it offers potential solutions to the so-called "small-scale controversies" associated with the standard cold dark matter (CDM) model while retaining agreement with well-established constraints on large-scale structure. FDM can originate from non-QCD axions with extremely small particle masses, $\sim 10^{-22}$ eV, and thus is in a state of Bose-Einstein condensation. Such non-QCD axions, dubbed axion-like bosons, can be one of the low-energy manifestations of String Theory. The major contribution of the NTU team includes the discovery of (a) stable solitonic cores that arise naturally from cosmological FDM perturbations [2.3.1], (b) relations between solitons and their surrounding dark matter halos [2.3.2], and (c) the unique random walk excursions of solitons [2.3.3]. This series of pioneering works published in Nature Physics and Physical Review Letters has received more than one thousand citations in the past six years. Clearly, the NTU team has been at the forefront of this field, with competition mainly from the Princeton, Columbia, and Gottingen groups.

Meanwhile, large cosmological magnetohydrodynamic simulations in the CDM model, such as IllustrisTNG [2.3.4], have proven extremely successful is modelling the evolution of large volumes of the Universe over cosmic time These models are now the primary method by which structure and galaxy formation theories are tested against data from the real universe. In comparison, even state-of-the-art FDM simulations cannot yet resolve a Milky Way-sized galaxy due to the high numerical expense caused by its wave nature. Nationwide collaboration in Taiwan underpinned by investment in HPC infrastructure and training is thus key to stimulating groundbreaking progress in FDM, especially because of the necessity to incorporate baryonic physics into the next-generation FDM simulations. This will enable FDM predictions of small scale structure visible in 21-cm intensity maps and Lyman-α forest power spectra in the post-reionization era, which will be powerful tools for distinguishing different dark matter models. Comparing the formation of first stars and the assembly history of first galaxies between the FDM and CDM scenarios will shed light on the cosmic phase transition of the early universe after the Big Bang and predict useful observational signatures for the forthcoming telescopes.

(2) Galaxy Formation and Evolution

Galaxy formation theorists study a complex network of astrophysical processes, from the evolution of the cosmic web of dark matter across the 14 billion-year history of the cosmos, to the nuclear reactions that govern the life and death of individual stars. Our understanding of the galaxy population as a whole has been revolutionized by multi-year survey observations on large telescopes that produced homogenous datasets for tens of millions of galaxies, such as the Sloan Digital Sky Survey. Theorists have developed a framework to connect these observations of the large-scale structure of matter in the universe and the statistical properties of the galaxy population to underlying astrophysical theory, such as stellar evolution, gravitational dynamics and the growth of supermassive black holes. The creation of 'mock galaxies' and 'mock universes' using large supercomputer simulations has been a fundamental theoretical contribution to this effort.

We now have a broad outline of the cosmic history of galaxy formation and knowledge of which astrophysical processes drive the phenomenology of the galaxy population. However, theoretical work to date has focused either on idealized small-scale physics (such as star formation in a tiny patch of interstellar medium with non-cosmological boundary conditions) or else on cosmological simulations, which necessarily abstract away most astrophysics on sub-galactic scales. The next major frontier in the subject is to bridge that gap by modelling sub-galactic astrophysics in detail. Key problems in this domain include the formation of stars from turbulent molecular clouds, the dynamics of the gaseous interstellar medium (ISM), and the flow of gas into and out of galaxies over cosmic time. A deeper understanding of this "baryon cycle" from simulations would, in turn, eliminate the presently intractable limit on small-scale tests of the nature of dark matter and the formation of the very first stars and galaxies. Modeling efforts that bring together specialists in all aspects of galaxy formation theory to bridge the 'sub-galactic gap' are therefore one of the clearest avenues for progress in the coming years.

Theoretical progress will be essential, because the community is facing a deluge of data in the next decade. Galactic astronomy will continue to be driven by the statistical power of survey observations such as ALMA and Subaru (HSC/PFS), with which both observers and theorists in Taiwan are already heavily engaged, as well as new facilities such as the Dark Energy Spectroscopic Instrument and the Vera Rubin Telescope. ALMA and JWST and future 30-m class optical telescopes will also deliver extremely high-resolution data on the sub-galactic dynamics of stars and gas for significant samples of individual galaxies. In this domain, theorists often work very closely with real data, either as members of small, fluid teams investigating specific objects or phenomena, or as part of large international collaborations structured around survey observations. Visibility and mobility within those collaborations are therefore vitally important for engagement of the Taiwanese community with this effort.

The following paragraphs briefly outline some key challenges in galaxy evolution in which Taiwan is well placed to make a significant impact. The computational astrophysics community in Taiwan has considerable expertise in these areas and is well-placed to develop numerical techniques and theoretical models that will be vital to interpret new data and plan for future facilities. Taiwanese researchers, many working overseas, already have important roles in major collaborations around each of these topics. The danger ahead is that, without investment to address the weaknesses outlined in the table above, the Taiwanese community as a whole may not fully benefit from, or not be fully acknowledged for, its contributions to this science.

Understanding the stellar initial mass function from first principles: this is a longstanding 'missing link' in the theory of star (and hence galaxy) formation theory [2.3.5]. Progress would open up a new era of galactic chemical evolution models in which the ISM is simulated in realistic galactic environments, evolving over cosmic time. Including the formation and evolution of interstellar dust self-consistently in such models would enable a further leap forward in understanding the observational properties of galaxies at ultraviolet to millimeter wavelengths. The Taiwanese community has well-established strengths in a number of fields related to this important problem (e.g. at NTNU, ASIAA and NTHU) that would benefit from greater collaboration around computational expertise and resources.

Energetic feedback from compact objects to the ISM: Feedback, arising from a wide variety of sources including stellar winds, supernovae and supermassive black holes (SMBHs), is an essential ingredient of galaxy formation theory but remains poorly understood [e.g. 2.3.6, 2.3.7, 2.3.8]. In addition to these sources, cosmic rays (CRs) have recently been shown to be an important ingredient missing from previous generations simulations that could have a significant impact on galactic winds driven by supernovae and the relativistic jets of SMBHs. Multi-wavelength data with unprecedented spatial and spectral resolution is expected to unveil new details of how feedback processes operate to regulate star formation on galactic scales, including a new generation of studies of the warm circumgalactic medium with quasar absorption spectra and x-ray observatories. This is a rapidly developing area in which groups at NTHU and ASIAA have recently hired specialists and hence are well placed to lead.

The growth and galaxy-wide impact of supermassive black holes: the details of CR transport depend on their interactions with the magnetic field on scales orders of magnitude smaller than the sizes of galaxies. Similarly, understanding of how supermassive black holes grow and release energy to affect their host galaxies has been hampered by the enormous gap in scale between galaxy population simulations on a cosmic scale and General Relativistic Magnetohydrodynamics (GRMHD) simulations on black-hole horizon scales. Innovative methods to bridge the gap and incorporate the microphysical processes are highly sought after. In Taiwan, a number of new faculty hires have expertise in modeling microphysics (NTHU), GRMHD theory and simulations (NTNU), and efficient GPU algorithms (NTU). Collaborations in this area have already been initiated within the TCA. Future faculty and postdoc hires as well as student training in synergy with this goal would build on this strength and promote Taiwan's distinctive role in this frontier research area.

Integrated models of galaxy formation: breakthroughs in the areas above will require developing sophisticated and comprehensive theories, implementing innovative algorithms, and conducting massive simulations. Since all of these topics are interconnected, they will eventually need to be modelled simultaneously, in integrated simulations evolved over cosmic time. Fortunately, many of the current members in TCA have complementary expertise, and collaborative work is ongoing. For example, the GPU-accelerated algorithms in GAMER can overcome a performance bottleneck currently holding back simulations of CR physics. In addition, due to the similarities between the numerical methods involved in CR physics and neutrino physics, code optimizations will benefit from joint efforts ongoing at NTHU and ASIAA. The physical insights gained from simulations that incorporate microscopic physical processes will be an important input for the semi-analytical galaxy formation models developed at NTHU and ASIAA, including dust formation and evolution in the ISM (Figure 4, top right). However, in spite of notable existing expertise, the Taiwan community currently lacks specialists in very large cosmological simulations that could make good use of NCHC, particularly with widely-used galactic hydrodynamical codes such as AREPO and GADGET4 [2.3.9]. Further hiring in this area is encouraged and would be of broad benefit to the galactic astrophysics community.

(3) Multimessenger Astrophysics

Recent multimessenger astrophysics (MMA) discoveries, including the co-detections of gravitational waves (GWs) plus electromagnetic (EM) waves [2.3.11, 2.3.12] and EM waves plus high-energy neutrinos from multimessenger sources [2.3.13], reveal valuable and unique insights into the physical processes and properties of many astrophysical phenomena. The combined observations from multiple messengers such as photons, neutrinos, gravitational waves (GWs), and cosmic rays enable us comprehensively to examine the underlying physics from a single multimessenger source. We have identified the following as key research directions that will combine current and upcoming EM waves, neutrino, GW, and cosmic-ray detectors (see Figure 4, bottom left) to enable exciting new discoveries in the next decade [2.3.14].

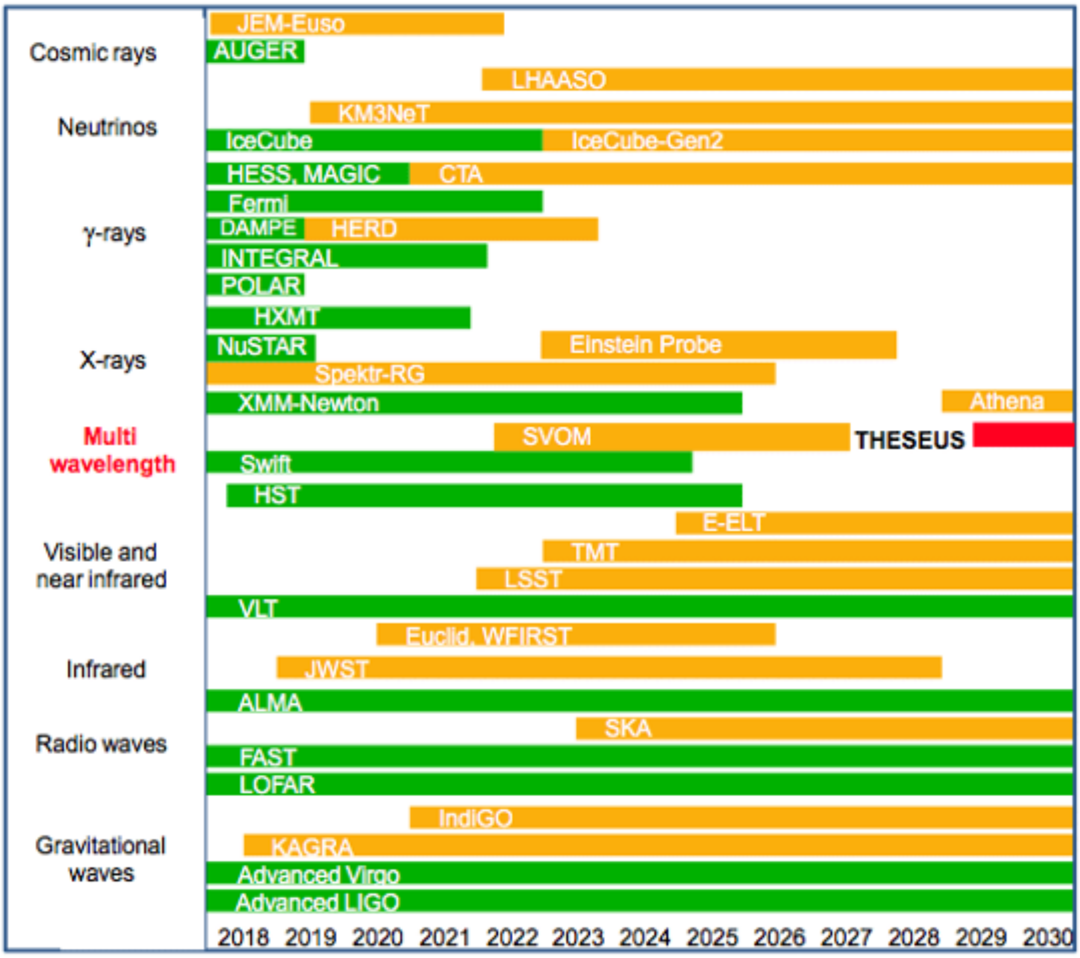

Figure 5. *The context of multimessenger Astrophysics in 2020-2030. Green and orange labels respectively indicate instruments currently operating and planned for the near future (as of 2018), respectively. Figure credit: S. Schanne [2.3.10].*

Important MMA research directions in the next decade:

Compact objects and energetic astrophysical phenomena, including supernovae, mergers of compact objects, supermassive black holes, active galactic nuclei, tidal disruption events, and fast radio bursts, will remain the primary sources of MMA in the near future.

The Kamioka Gravitational Wave Detector (KAGRA) has joined the third observation run (O3) together with the Advanced LIGO and Advanced Virgo in early 2020. The newly established network, with four GW detectors, will improve the localization volume in O4 (2022-2023) by a factor of two over that of O3 [2.3.15]. The individual updates of each GW detector could further increase the rate of event detections in O4 by roughly one order of magnitude. In 2025, the fifth ground-based GW detector, LIGO India, will join the network, significantly improving the detections and localization and helping to optimize multimessenger follow-up source identification. In addition, the coming Vera Rubin Telescope (formerly the Large Synoptic Survey Telescope,LSST) and the Roman Space Telescope (formerly WFIRST) will discover a tremendous amount of new multimessenger transients with much better temporal sampling, image depths, and sky coverage. The next generation low- and high-energy neutrino detectors, such as Hyper-Kamiokande and IceCube-Gen2, will collect roughly ten times more neutrino events than existing detectors. Combining all these upcoming facilities, the expected future multimessenger detection of EM waves, GWs, and neutrinos will be able to shed light on the as-yet-unknown mechanisms of different classes of supernova explosion, the origin of elements, the properties of ultra dense matter, and the accelerated expansion of the Universe ascribed to dark energy. These data also have important implications for particle physics, including the properties of neutrinos, the origin of ultra-high-energy cosmic rays, and the nature of dark matter.

In addition, after the first black hole image released by the Event Horizon Telescope collaborations, a next generation Event Horizon Telescope (ngEHT), founded by the National Science Foundation (NSF), is under design [2.3.16]. With increased ground telescope sites and observational frequency bands, ngEHT will reveal the nature of more black hole systems and bring better understanding of the jet launching and accretion physics. Especially, with the accumulation of knowledge for both the horizon-scale ($\leq 10\ R_g$; $R_g = GM/c^2$) and large-scale (e.g. $>10^5\ R_g$) physics of relativistic jets, several important theoretical topics across different length scales can be pursued in MMA: jet launching, jet acceleration, generation of high-energy gamma-ray emission and neutrinos within the jet, interaction with ambient environment, and the feedback to the host galaxy etc.

Current status and previous achievements:

Theoretical and computational multimessenger astrophysics in Taiwan has received a boost in recent years due to new faculty hirings in several universities and institutes, including ASIAA, ASIoP, NTHU, and NTNU. Individual research groups focus on the modeling of supernova explosions and their multimessenger observables, the astrophysics and physics related to merger of compact objects, as well as simulations of supermassive black holes - accretion disk systems. Several ongoing collaborations between theory groups are being carried or planned; e.g., magneto-hydrodynamic supernova simulations coupled with advanced neutrino transport; combined analysis of multi messenger signals from different sources; simulation of neutron star merger outflows coupled with nuclear reaction network; the connection between high-energy neutrino emission from black hole-accretion disk systems and the underlying engine properties. Meanwhile, an increasing number of groups in Taiwan (ASIoP, NCKU, NCU, NTHU, NTNU, and TKU） have joined the KAGRA collaboration to work on different topics related to gravitational wave astronomy. Opportunities of further coordinated work may thus be expected with the platform provided by the NCTS. Furthermore, synergetic efforts between theorists and observers in e.g., the Event Horizon Telescope (EHT) and Greenland Telescope (GLT) collaborations, ALMA, Pan-STARRS, Global Relay of Observatories Watching Transients Happen (GROWTH) and the Compton Spectrometer and Imager (COSI), will maximize the dynamics and the scientific impact of Taiwan's astronomy community. Beyond pure astrophysics, interdisciplinary efforts involving communities of e.g., particle cosmology & astroparticle physics (TG2.1), gravity theory (TG2.2), and the development of advanced instrumentation can further enhance the development of multimessenger astrophysics.

Future strategy:

Given the current status described above, we expect that the multimessenger astrophysics community in Taiwan can continuously deliver impactful scientific outputs in the next decade for a majority of the important topics we have identified. Nevertheless, several improvements to the community can still be made. Our two key recommendations for the multimessenger astrophysics community in Taiwan are as follows.

1. Strengthening existing teams

   It is important to provide continuous support to existing strong teams at the above institutions, not only to help them grow, but also to reinforce the cross-team collaborations. To achieve this goal, it is critically important to hire qualified postdocs and to cultivate PhD students who can work together with more than one PI. Postdoc fellowships supported by the NCTS are ideal for this purpose. For students, programs involving multiple institutes may need to be established, with advanced training provided through the joint force of NCTS and participating institutes.

2. Enhancing synergetic efforts between theory and observation

   Although strong joint forces between theory and observation are already established in particular subfields (e.g., EHT), it is critical to further enhance the connection of theory predictions to the upcoming observational data, and to expand/link the scientific strength to other wavelengths/messengers (e.g. exploring X-ray polarization properties of black hole - accretion disk systems; in contrast to the EHT observation at the radio band). The current multimessenger community is particularly lacking expertise in i) detailed radiative transfer modeling (key to predict multi-wavelength lightcurves/SEDs), and ii) in-depth Bayesian analysis (traditional or machine learning) founded on expert knowledge of both theory and observation. Future faculty recruitments targeting this expertise would strongly reinforce the vital theory-observation connection.

In addition to these two key recommendations, further emphasis on the development of state-of-the-art, high performance tools (e.g. GPU-based GRMHD codes, GPU-based General Relativistic Monte-Carlo radiative transfer codes) is highly encouraged, as is the hiring of experts who work on numerical simulations related to multi messenger topics. Future success in this field will also depend on investment in computational resources and the development of new simulation tools, which will be addressed in Section (e) below.

(4) Planet formation

Planet formation and evolution are expected to remain one of the most rapidly developing fields in astronomy over the next decade, thanks to instruments such as ALMA and future missions such as JWST (2021), PLATO (2026), ARIEL (2028), etc. These will generate a tremendous amount of observational data on exoplanets as well as their formation environment — protoplanetary disks (PPDs), which will require detailed theoretical models for interpretation (Figure 4, bottom right). We identify two major directions for the Taiwanese community:

1. <u>Connecting planet formation to star formation and satellite formation</u>

   Current observations of PPDs suggest planet formation may take place earlier than previously thought [2.3.17, 2.3.18]. This implies that planet formation is intimately linked to the formation of stars and their surrounding PPD. At the same time, future high-resolution observations are expected to provide ever-more detailed information on exo-planetary atmospheres, circum-

planetary disks, and possibly exo-moons. An inevitable trend in planet formation is thus its evolution into a *multi-disciplinary* problem in connection to the above topics that occur on both larger and smaller scales.

At larger scales (up to star-forming clumps of a few pc), only a handful of numerical simulations have treated the formation of proto-planetary disks in a self-consistent way during the formation of stars in a diffuse turbulent interstellar environment. For example, recent work by the NTNU group demonstrated that the disk in its embedded phase is significantly different to later stages, where the disk can be treated as an isolated entity, and therefore significant model revision of the early dynamics of the PPD is to be expected [2.3.19].

Going down to planetary surroundings, the modeling of atmospheric activities of small Solar System bodies in response to their ambient plasma environments and the Solar radiation is a probe to their interior composition, which are intimately linked to the history of the planetary system. As an example, Europa has a tenuous atmosphere produced by plasma sputtering, sublimation, and thermal desorption. The atmospheric composition is hence closely related to the surface and possibly interior (oceanic) material from outgassing activities. (NTNU has been actively involved in such studies.) Such features have also been found on Mercury, Moon, Dwarf planets (i.e., Ceres), and satellites in the outer Solar System. Such models are directly applicable to the studies of exo-planetary systems in the future.

2. Connecting theoretical models with observations

Planet formation is and will remain an observationally-driven field for the foreseeable future. Theorists must therefore be able to explicitly relate models to observables. For example, it is becoming increasingly common to produce synthetic ALMA observations along with simulations of PPDs [e.g. 2.3.20]. There is some effort in this direction through the CHARMS initiative at ASIAA, but overall a direct interface between theory and observations is lacking in Taiwan. The dissonance between theory and observation is a major weakness of Taiwanese research in planet formation theory.

There are also existing Taiwanese groups (namely NCU, NTNU) that study the Solar System based on extraterrestrial samples (cosmochemistry of meteorites) and measurements from space missions (e.g. CASSINI). Such laboratory or in-situ measurements strongly constrain the present-day appearance of the Solar System, and thus its history as well. Simulations of the cometary jets and outgassing plumes of the icy satellites are necessary for understanding the interior structure of such small bodies that preserve information from the first millions of years of the Solar System.

Theoretical planet formation in Taiwan is in its infancy with only a few faculty at ASIAA and NTNU, some of which are relatively recent hires. However, star formation and planetary sciences (including Solar System studies) have been traditional focuses at several institutes already, e.g. ASIAA, ASIES, NCU, NTNU. We thus recommend both expanding Taiwan's theoretical planet formation community and its tight integration with established groups in star formation and planetary sciences by taking advantage of the NCTS platform. Theorists should take advantage of Taiwan's deep involvement with observational studies of PPDs and the Solar System and apply their models to real data.

The top priority is to hire new faculty and lead the above fields. For 1), experts in hydrodynamics, magneto-hydrodynamics, N-body dynamics, and direct simulation Monte Carlo are needed. Background and experiences in star formation, Solar System dynamics, or both, are desirable. For 2), observationally-orientated theorists are needed, including experts in radiative transfer, astrochemistry, synthetic observations, and population synthesis. The next priority is to hire postdocs in these areas to sustain a stable research output. Finally, students should be trained with interdisciplinary directions, e.g. they may be encouraged to take classes from physics, earth sciences, and atmospheric physics, and partake in both theoretical and observational projects during their studies.

We also suggest synergetic programs to support 1) and 2). This includes joint-postdoctoral fellowships, workshops, and schools between different institutions, or between different groups within the same institution. For 2), we recommend training current and future theorists to work with observers and observations. Academic activities, at least initially, should be targeted at finding common interests. Joint and interdisciplinary research as described above should be supported.

(5) Infrastructure for computational astrophysics

HPC is an indispensable tool for theoretical astrophysics. It is equivalent to telescopes for observational astronomy, and theoretical astrophysics has traditionally been a leading driver of scientific HPC development[3]. The overall direction of scientific computing in the next decade will be defined by the transition to exascale computing and the continual rise in the use of GPUs for scientific simulations and analysis. *If Taiwan is to remain internationally competitive, we must improve the provision of hardware and software and strengthen collaboration between research scientists and experts in scientific computing. The idea of an integrated computational 'ecosystem' is key. Large investments in centralized facilities such as the NCHC will be ineffective unless there is also investment in the support and training that underpin day-to-day scientific computing work in university departments and research institutes, and so develops a sophisticated, internationally engaged user base (including PhD students and postdocs).* We believe the computational astrophysics community in Taiwan is now well placed to advise and support the funding agencies in strengthening support for mid-scale research HPC, because many recent faculty hires have decades of collective experience working in some of the world's leading computational astrophysics centers. We consider the following two points to be most critical to success in the short term. We remark that these are also applicable to realize the goals of TG4.

First, at present, there is no specific funding support for mid- and large-scale HPC resources. Researchers are limited to procuring individual small-scale machines or short bursts of computing time on NCHC through individual grants from the funding agencies. This makes it difficult to build up the momentum and expertise required to realize ambitious scientific projects or (in the case of theorists specializing in large-scale computation) to satisfy everyday needs. Often multiple PIs resort to consolidating their general grants from the funding agencies for these purposes. Such consolidation at the institute and department level is the international standard and vastly more efficient (financially and scientifically) compared to a 'one cluster per PI' approach. However, funding and support for institute-

[3] For example, computational astrophysics played a leading role in the development of the UK's main national scientific HPC infrastructure project, DiRAC (https://dirac.ac.uk). DiRAC has a substantial legacy of hardware and expertise from the Virgo Consortium, a highly successful collaboration between theoretical astronomy groups, founded in the late 1990s using national grant funding to develop cosmological and galaxy formation simulations (including the landmark Millennium Simulation). A notable feature of the Virgo Consortium was its support for full-time HPC experts and mid-scale HPC infrastructure within individual institutes, alongside support for postdoctoral researchers, large projects and academic exchanges.

scale HPC in Taiwan is almost non-existent, inefficient and limited in scope. This puts Taiwanese researchers at a significant productivity disadvantage compared to our international peers.

We therefore recommend new funding opportunities be developed, in partnership with the community, that would enable university departments and research institutions to procure and support in-house mid-scale HPC clusters as collective institutional projects. Smaller institutes could use the same framework to pool grants with larger institutes, or purchase time on NCHC or cloud computing services. In-house facilities, when properly funded and managed, can provide a tremendous productivity boost. Although national facilities like NCHC are vital for large 'production run' calculations, in-house facilities better serve everyday needs for software development, access and training for students and postdocs, and small-to-intermediate scale calculations. Funding for 'breakthrough' extremely large-scale, state-of-the-art simulations on NCHC, which might require tens of million core-hours and involve bespoke teams of researchers from different institutes, could be awarded to selected PIs through special competitive grants from the funding agencies or NCHC.

Second, there is also an urgent need to hire technical staff to support and develop HPC infrastructure at the departmental and institutional level. Although centralized national-level computing facilities are critical for the largest projects, technical support embedded within research groups is equally vital to the success of day-to-day scientific work. Expert staff working alongside researchers (with parity in salary and esteem) are a cornerstone of all the world's leading centers of theoretical astrophysics. They make an essential contribution to research productivity by exploiting the full capabilities of hardware and software, training researchers and students, and ensuring effective procurement. In other countries with a substantial astronomical research community, research computing support positions are centrally funded and highly competitive, despite salary levels well below those of industry.

We hope a scheme can be worked out to provide more incentives for attracting and retaining such staff within institutes and departments, including through the provision of secure, long-term positions that value their expertise. Since computing technology is an internationally recognized pillar of the Taiwanese economy, this could be a productive area to channel investment from industry into fundamental research, including computational astrophysics. We also recommend more faculty and postdoctoral hires that focus on software development (e.g. GPU codes), as there has only been one recent faculty hire in this area (at NTU). Supporting in-house computing to an international standard, both in hardware and personnel, will be an important part of attracting the best international researchers to Taiwan.

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TG3: Condensed Matter

The broad field of condensed matter physics has made possible the miracle of the silicon industry in Taiwan. It is also providing the answer to keep beating Moore's law when the traditional way of IC manufacturing seems to reach its limit. It addresses the question of how we can understand our material world from fundamental physical principles and quantum computations, and how we can use this capability to discover novel materials that may not exist in Nature to better our lives. It is also making quantum computing and quantum information technologies possible. Here we identify the following two TGs in the field. Not only the participants in these TGs will interact and collaborate, but also they will talk and collaborate with researchers participating in TG1 above and TG4 below..

TG3.1: Computational Quantum Materials Physics

(Discovery and Design of Novel Materials through *Ab Initio* Calculations)

Important directions in the next decade

In the next decade and beyond, with further advances in *ab initio* many-body theories beyond the density functional theory, numerical algorithms, machine learning, and faster computers, and especially new computing paradigms emerging on the horizon, *ab initio* calculations will play an ever increasingly important role in condensed matter and material physics. TG3.1 has identified the important research directions in the next decade:
(1) Two-dimensional materials
(2) Topological materials
(3) Method for studying strongly and intermediately correlated materials
(4) Machine Learning Guided Condensed Matter Research

(1) Two-dimensional materials:

The typical two-dimensional (2D) material Graphene may be one of the hottest fields in physics research [3.1.1]. It is a one-atom-thick 2D material with carbon atoms arranged in a single-layer honeycomb lattice possessing an unusual band structure with a linear dispersion, exhibits fascinating physical properties such as extraordinary mechanical strength, ballistic transport with charge carriers mimicking massless Dirac fermions, and supreme thermal conductivity. Thus, graphene has attracted enormous attention since it was isolated and characterized for the first time in 2004. The current interest in graphene has also stimulated research efforts to fabricate other 2D materials that could also show novel properties beyond graphene.

For example, since it is comparatively difficult to open an energy gap at the Dirac point and not easy to integrate into the well-developed silicon industry, there are increasing new 2D materials discovered for the next generation semiconductor industry in recent years. Indeed, many of them, such as graphitic BN layers, monolayers of group IV elements (silicene, germanene, etc.) and group III,V compounds (borophene, phosphorene, etc.) as well as transition metal dichalcogenides (TMD) (MoS_2, WSe_2, etc.) and Bi compounds, have been fabricated and characterized. These new 2D materials could exhibit a number of intriguing properties such as quantum spin Hall effect and nonlinear optical properties that the corresponding bulk materials do not have. They also have several promising applications such as novel types of transistors, efficient catalysts for hydrogen production, and spin transport devices.

One of the most exciting recent developments in 2D quantum materials is the discovery and characterization of magnetism and superconductivity in exfoliated single-layer materials. 2D magnetic layers such as CrI_3, $Cr_2Ge_2Te_6$, and so on, have attracted tremendous attention in recent years. The huge interest originates not only from the fundamental physics of how the forbidden 2D-long range magnetic order is established but also from the high potential in next generation storage devices. In combination with 2D or 3D superconductors, these developments pave the way for an enormous influx of new quantum materials designed layer by layer through mechanical stacking. Today, given the dramatic advances in nano-characterization tools driven primarily by the study of graphene, the science of 2D quantum materials is poised to advance very quickly. Here we propose to perform the state-of-the-art ab initio calculations in order to provide a theoretical understanding of the fundamental properties of these emergent low-dimensional materials and also to assess their application potentials.

Heterostructures are also important 2D systems since the 2D interfaces would lead to surprising new physics and provide more space for manipulation [3.1.2]. It has been intensively studied that there can be magnetism and superconductivity at the interface between different transition-metal oxides such as LAO/STO. There could also be very interesting phenomena such as 2D to 1D charge condensation and interface-induced ordering at the interface. Combinations of different van der Waals layers such as metal/topological insulators(TI), TMD/TI, TMD/graphene/magnetic layer, and so on, provide a much more wide spectrum for different possibilities[3.1.3, 3.1.4]. Furthermore, the growth of 2D iron-based superconductors ultrathin films or their cleavages from the bulk is also a part of the emerging 2D physics and surface physics.

Nano-structures such as nano-ribbon, metal cluster, TMD-flake, one-dimensional atomic chain, and so on, which belong to the system with dimensions lower than 2, are also an important research field. These kinds of systems show intriguing properties which are often out of expectation. For example it can become magnetic when a nonmagnetic material is down-sized to the nano-scale. On the contrary, a nano-structure composed of magnetic materials could show nonmagnetic behavior due to subtle interactions with the substrate. One-dimensional magnetic atomic chains can even host Majorana states for quantum computing. Recently zero dimensional single molecule electronics even show increasing potential in the next generation sub-nano industry owing to the stable structure with the smallest size that humans can manipulate.

(2) Topological materials:

Understanding fundamental physics in different phases of matter is one of the most important goals of condensed matter physics. Before 1980, the phase transitions of matter were mostly described by Landau phase transition theory, which is based on the concept of spontaneous symmetry breaking. When a system undergoes a phase transition, the symmetry of the system changes. However, in early 1980s, scientists noticed that the quantum Hall effect cannot be described by this Landau theory. The experiments show that the integer jumps in Hall conductance caused by a varying magnetic field are not accompanied by any symmetry changes of the system. The key to understand this extraordinary phenomenon lies in the fact that the Bloch state wavefunctions can be mapped to a manifold in the projective Hilbert space. For systems like the quantum Hall systems, this manifold has a nontrivial topological structure. Because of the discovery of this hidden intriguing topology in the manifold of the electronic quantum states by Nobel Laureate David J. Thouless and others, we now have a fuller understanding of phases of matter which goes far beyond the Landau theory of spontaneous symmetry breaking [3.1.5]. Nevertheless, due to the limitations of the experimental technology at that time, neither the theoretical development nor the experimental advance led scientists to discover real materials with a nontrivial topology. Soon after the graphene was made by mechanically exfoliating graphite by Nobel Laureates Konstantin Novoselov and Andre Geim, Charles Kane and E. J. Mele predicted that Dirac semimetal graphene would become a 2D topological insulator if the spin-orbit coupling is taken into account [3.1.6]. This ushers in the current exciting age of topological materials in which the concept of topology of quantum states takes a center stage.

Before 2010, the research effort was mainly placed on topological insulators (TIs). Three-dimensional (3D) TIs are distinct from the conventional band insulators in the sense that they feature a bulk energy gap driven by spin-orbit coupling effect and gapless surface states protected by time-reversal symmetry. The surface states in TI are topologically protected and immune to impurities or geometric perturbations, which are distinct from the surface state of semiconductors that can be removed by any surface perturbation such as an external field. Inside such a TI, Maxwell's laws of electromagnetism are dramatically altered by an additional topological term with a precisely quantized coefficient, which gives rise to remarkable physical effects. In the past decade, many new topological phases beyond TIs have been identified, such as topological semimetals, topological crystalline insulators, as well as topological superconductors (TSCs). Besides nonmagnetic systems, the interplay between topology and magnetism provides an opportunity to realize exotic physical phenomena, such as the quantum anomalous Hall effect and the quantized axion electrodynamics. Therefore, the topological magnetic materials have currently emerged as a frontier of the field. Now topological materials have developed into the most important branch of condensed matter physics.

Let us now briefly introduce the two most important applications of topological materials. First we introduce the axion electrodynamics time-domain terahertz (THz) polarimetry on time-domain terahertz polarimetry. Terahertz is considered a radiation source with many unique advantages. For example, this spectral region contains very rich physical and chemical information in matter. Moreover, the data transmission speed of THz-Wi-Fi is expected to reach 100 Gbit/s. Therefore, the development of THz technology is a very important cross-cutting frontier for technological innovation or national economic development. Terahertz radiation occupies a middle ground between microwaves and infrared light waves, known as the "terahertz gap", where technology for its generation is in its infancy. In addition, terahertz radiation can penetrate thin layers of materials but is blocked by thicker objects. As a consequence, the generation and modulation of electromagnetic waves in this frequency range ceases to be possible by the conventional electronic devices used to generate radio waves and microwaves, requiring the development of new devices and techniques. Recent work proposed the observation of quantized Faraday and Kerr rotations of THz in TI thin film under a strong external magnetic field [3.1.7]. This finding indicates that TI is a candidate material that can be used to manipulate THz in the nanoscale. However, strong magnetic field equipment limits the size of the devices. In the early of 2020, intrinsic magnetic topological materials have been realized. Latest research work predicted that the topologically nontrivial surface gap on the surface of magnetic topological material possesses half quantized axion coupling, which will modify the Maxwell equation by an additional topological axion term. This additional charge and current terms may interact with THz radiation, realizing the manipulation. Because the magnetic topological material has inherent internal magnetic moment, there is no need to generate an external magnetic field by a huge external magnet. As a result, the size of the devices can be greatly reduced. Another important application is about quantum computing. Quantum technology has been regarded as a major technological development by countries all over the world, and quantum computing is the focus of recent developments (see TG1 above). Very recently, IBM and Google proposed their quantum computers with about 53 and 72 qubits, respectively. Different from an existing superconducting qubit, topological qubit is another way to realize quantum computation. The advantage of the topological qubit lies in robustness. In principle, as long as the external perturbation does not close the energy gap of the topological system, the topological qubit will not be eliminated. Therefore, compared with existing methods, this type of quantum computers possesses a higher fault tolerance rate. On the surface, the topological qubit seems impeccable, and this is why Microsoft chose this way. However, the biggest problem is that there is no experiment to produce any real topological qubit yet. Generating Majorana fermion (MF) is the most important step in realizing topological qubit. It is currently recognized that the observation of these three experimental signals can prove the existence of MF: zero-bias peak, half-integer quantum conductance, and non-abelian statistics. Since the 1997 theoretical model was proposed, many experimental groups have observed zero-bias peaks in different systems. The Microsoft group even observed integer zero-bias voltage peaks in 2018. At the same time, the experimental signal of half-integer quantum conductance was also observed by the UCLA group in 2017. It seems that the realization of MF is close at hand, only the last step of non-abelian statistics. However, in March 2021, Microsoft retracted their *Nature* paper [3.1.8]. The integer zero-bias-peak that they observed have systematic correction errors. On the other hand, the half-integer quantum conductance observed by UCLA has been controversial since the article was published. Therefore, it is still a long way to realize the topological qubit.

IBM and Google have produced a considerable number of qubits. It is often difficult to surpass the existing groups in the world in this regard. But for the topological qubit, to the advantage, Taiwan and other groups in the world are equal (there is no group that has ever produced topological qubits). Taiwan has accumulated a certain amount of research energy in topological materials in the past 10 years. Several theoretical and experimental groups have invested in it for a long time. In addition, the Taiwanese group observed the signal of a topological superconductor in 2017, and also observed a zero-bias peak in the superconducting energy gap. Taiwan is not completely inexperienced in this area, thus investing in this area may have an opportunity to achieve the world's leading position.

(3) Correlated materials:

We identify three subfields in *ab initio* study of correlated systems and excited state physics.

(a) New functional for systems with weak to intermediate correlations. The success of DFT relies largely on the computationally effective and accurate exchange-correlation functionals. For simple metals and *sp*-electron semiconductors, the local density approximation (LDA) and generalized gradient approximation (GGA) prove to be the working horse. Nonetheless, in transition metal oxides, *d*-electrons are often strongly correlated and are difficult to treat. Similar problems are also observed in some 2D transition metal sulfides and Fe-based superconductor FeSe, where the computed bandwidth may be overestimated. Newly developed SCAN functional [3.1.9] shows promising improvement over LDA or PBE on some properties of prototypical ferroelectric, Si, and water molecules with a cost less than the hybrid functionals. It provides an alternative to the commonly used LDA/GGA+U scheme with an *ad hoc* Hubbard U term [3.1.10]. However, it overestimates magnetic moment of itinerant electron ferromagnets like bcc-Fe, fcc-Ni, and hcp-Co and shows numerical instability in certain cases. A continuing development of new functionals is an indispensable direction in material sciences. The same effort in designing new functionals has also been emphasized in the chemical physics society. Researchers in this direction could synergize well with TG4.2a.

(b) For strongly correlated materials, although LDA/GGA+U could occasionally give correct band structure, magnetism, and charge-orbital orders in many transition metal oxides, it fails to describe the spectra at finite temperatures and magnetic transitions. For example, high temperature superconductor parent compound La_2CuO_4 is an antiferromagnetic insulator at low temperature and becomes a paramagnetic insulator above the transition temperature. Since dynamical local correlations are completely neglected in LDA/GGA+U, a more accurate method is necessary. Latest research has shown that a combination of GW and DMFT, which takes into account both long-range dynamical correlations and accurate local dynamical one, could be a possible route to deal with strongly correlated materials. Recent results show that GW+DMFT method can capture essential correlations in Fe-based superconductor LiFeAs observed in the ARPES experiment [3.1.11, 3.1.12].

(c) Excited state physics. Excited state properties of materials are not only directly related to their application values but also important fundamental questions in condensed matter physics. For example, excitons, which are bound electron-hole pairs, are crucial in light-matter interactions. Understanding their properties is the key to design better photovoltaic and optoelectronic devices. First-principle calculations on the exciton properties can now be performed routinely with a reasonable amount of computational resources. However, *ab initio* study on other exciton complexes like trions and bi-excitons, which are important in doped or highly excited semiconductors are still out-of-reach. With the advancement in computational power and further development in theory and computational tools we believe that a better understanding of these exciton complexes should become possible soon. At the same time other quasi-particles such as plasmon, polaron, and polariton which play important roles in light-matter interaction, quantum transport, and energy transfer, can now be studied with *ab initio* methods. Along this direction efforts have also been put on developing first-principle quantum dynamic simulation tools, which in principle can cover all excited state properties and allow us studying nonequilibrium phenomena observed in ultrafast experiments [3.1.13].

(4) Machine Learning Guided Condensed Matter Research

In recent years, huge amounts of theoretical and experimental data in several fields of study have been constantly produced. In the field of computational materials science, the abundance of data is due to the success of density functional theory (DFT), along with high-throughput (HT) approach, and the development of faster computers. Also, advances in the field of instrumentation and electronics have enabled experiments to produce large amounts of data. The amount of data being generated by simulations and experiments has led us to the fourth paradigm of science, the (big) data-driven science. Such a paradigm naturally follows from the first three paradigms: (i) experiment, (ii) theory, and (iii) computation/simulation, as shown in Figure 5. Its impact in the field of materials science has led to the emergence of the new field of materials informatics. To take advantage of this vast amount of information, the development of techniques that would enable the extraction of knowledge from such data is the most logical step to pursue. One of the tools that is currently steering research into a new data driven science paradigm is Machine Learning (ML).

Established methods to theoretical and computational materials science depend on the calculation of properties based on the atomic structure and composition of materials. Thus, searching for candidate materials for desired applications can be a laborious process. The possibilities will be restricted based on the researcher's prior knowledge about similar materials. With the advancement of computational science, this trial-and-error approach has now been improved and supported in an attempt to lessen the search area. Still, the resulting tremendous amount of generated data provides no assurance that this will lead to usable information and knowledge. Moreover, the ultimate goal of applying this knowledge for the benefit of the human race is an even larger challenge. Therefore, the usage of ML techniques is of utmost importance in order to reduce the knowledge gap and enhance materials research under our current situation.

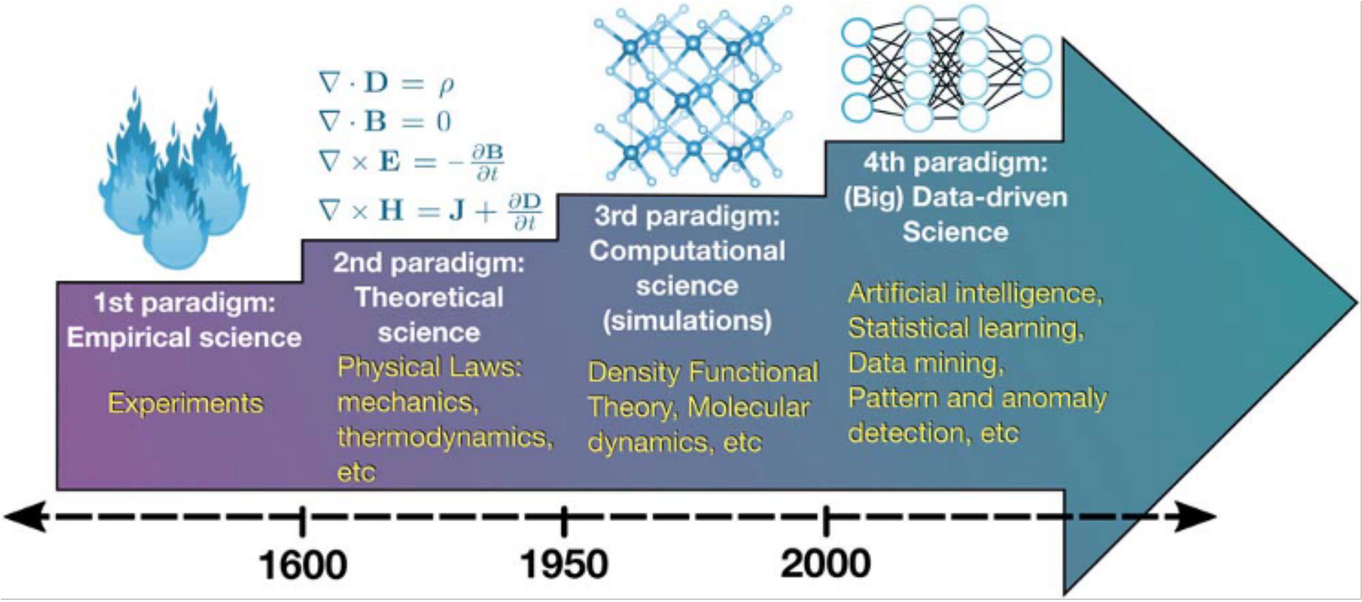

Figure 5. Recent development in data-driven research gave rise to the fourth science paradigm: (i) empirical, (ii) theoretical, (iii) computational, and (iv) data-driven. Each paradigm is dependent on each other in a beneficial way [3.1.14].
https://doi.org/10.1088/2515-7639/ab084bhttps://doi.org/10.1088/2515-7639/ab084b

The utilization of ML techniques to materials design and discovery includes the determination of crystal structure, properties, and parameters of unknown or complex materials. Optimization methods such as High-Throughput method, Genetic algorithm, Greedy algorithm, Random search algorithm, Gradient descent methods algorithm, neural network are the candidate approaches to be used in this study.

The accuracy of material property prediction is highly reliant on the methods of calculation which span quantum mechanics, tight-binding models, and force-field methods. To perform large-scale calculations for complex materials, computationally expensive methods based on DFT is not feasible. Traditional methods for parameterizing these parameters to accurately reproduce the results from quantum mechanics are slow and tedious. Therefore, using ML methods, such as Genetic algorithm and Neural network, to optimize the best parameters for large scale simulations is highly demanded.

Strengths and opportunities for Taiwan:

Taiwan is one of the major manufacturers of personal computers and components in the world. However, due to the limitation of the working population of Taiwan, the number of researchers are not as many compared to nearby countries such as Korea, Japan, and China. Nevertheless, there are quite a few at the faculty level scattered in several institutions all over the country. These outstanding *ab initio* condensed matter theorists are research pioneers in their own respective fields. Therefore, our chief purpose is that, in the framework of the NCTS, we will coordinate our individual efforts, and concentrate our limited manpower and resources to tackle the few most relevant issues in condensed matter and materials physics, and strive to make some breakthroughs. Together, we will also train our young materials physicists to maintain leadership in certain important research directions. Moreover, we will work closely with our experimental partners, as well as interact and collaborate with our overseas colleagues.

(a) Talents in Taiwan:

The following researchers are the talents of this computational condensed matter physics in Taiwan: the core members of TG3.1 in the current phase are Tay-Rong Chang (NCKU), Yang-Hao Chan (IAMS, Academia Sinica), Feng-Chuan Chuang (NSYSU), Guang-Yu Guo (NTU), Horng-Tay Jeng (NTHU), and Hsin Lin (IOP, Academia Sinica). Other talents include Mei-Yin Chou (IAMS, AS), Ching-Ming Wei (IAMS, AS), Chi-Cheng Li (TKU), Hung-Chung Hsueh (TKU), Ming-Hsien Lee (TKU), Chih-Kai Yang (N Chengchi U), Tsan-Chuen Leung (N ChungCheng U), Han Hsu (NCU), Yu-Hui Tang (NCU), Yu-Chang Chen (NYCS), Bi-Ru Wu (CGU), Chun-Ming Chang (NDHU), Chun-Wei Pao (RCAS, AS), and Chao-Cheng Kuan (RCAS, AS).

(b) Recommended strategy and teams to watch

The research direction of each core member will focus on their expertise, and each team can collaborate with each other to maximize the efficiency and benefits of TG3.1. We also plan to hold workshops and conferences to increase the opportunity of collaborations between groups and to provide training for new students and postdocs. With regard to international collaborations, many of the talents listed here already have world-renowned long term collaborators. We will invite them to visit NCTS and strengthen these collaborations. To set foot in the new direction, we hope to send students to leading international research institutions. We highly recommend the group leaders to encourage the young scholars in their groups to expose themselves to international collaborations. Physicists with excellent programming skills are crucial to TG3.1. Extensive training in programming is needed.

(1) Two dimensional materials

Taiwanese researchers were quite active in the field of surface physics and interface during the 1990s. The research groups in Taiwan have quickly shifted from surface physics to 2D materials since the emergence of 2D materials beyond 2005. There are already internationally recognized and famous research groups in Taiwan. The research group in Academia Sinica is one of the concentrated institutes focusing on surface physics and 2D materials led by Mei-Yin Chou (IAMS, AS) and Ching-Ming Wei (IAMS, AS). Furthermore, other groups in Taiwan include Feng-Chuan Chuang (NSYSU), Tay-Rong Chang (NCKU), Horng-Tay Jeng(NTHU), Guang-Yu Guo(NTU), Hsin Lin(IOP, AS), Chih-Kai Yang (NCCU), Tsan-Chuen Leung (NCCU), Chao-Cheng Kaun (RCAS-AS), Han Hsu (NCU), and Yu-Chang Chen (NYCU).These groups have different collaboratively experimental groups to collaborate internationally and locally.

Teams: Mei-Yin Chou (IAMS, AS), Ching-Ming Wei (IAMS, AS), Feng-Chuan Chuang (NSYSU), Tay-Rong Chang (NCKU), Horng-Tay Jeng (NTHU), Guang-Yu Guo (NTU), Hsin Lin (IOP, AS). Chih-Kai Yang (NCCU), and Tsan-Chuen Leung (NCCU).

(2) Topological Materials

The research on topological materials was initiated in 2005, but it started to spread in a small research community before 2011. The research topics then were introduced to Taiwan around 2011. After that, numerous groups in Taiwan have established their own research credential globally. These groups include Feng-Chuan Chuang (NSYSU), Tay-Rong Chang (NCKU), Horng-Tay Jeng (NTHU), Guang-Yu Guo (NTU), Hsin Lin (IOP, AS). Our core members are all world famous researchers in the field of topological materials.

Teams: Feng-Chuan Chuang (NSYSU), Tay-Rong Chang (NCKU), Horng-Tay Jeng (NTHU), Guang-Yu Guo (NTU), and Hsin Lin (IOP, AS)

(3) Correlated materials

Guang-Yu Guo (NTU), Horng-Tay Jeng (NTHU), Hung-Chung Hsueh (TKU), Chi-Ming Wei (IAMS) are experts in +U and GW-BSE methods for excited state calculations. Shih-I Chu (NTU) is a leader in the development of time-dependent dynamics of many-electron quantum systems. In addition to the existing talents mentioned above, new faculty members Chi-Cheng Lee (TKU) and Yang-hao Chan (IAMS, AS) are also actively working on first-principle excited state physics.

Teams: Guang-Yu Guo (NTU), Horng-Tay Jeng (NTHU), Hung-Chung Hsueh (TKU), Chi-Ming Wei (IAMS, AS), Chi-Cheng Lee (TKU), and Yang-hao Chan (IAMS, AS)

(4) Machine Learning Guided Condensed Matter Research:

Feng-Chuan Chuang (NSYSU) is a leader in developing efficient methods for atomic structure optimizations using Genetic algorithm, Greedy algorithm, Basin-hopping, and High-Throughput approach. Ching-Ming Wei (IAMS, AS) developed the basin-hopping algorithm (random structure search) to search for the atomic structures of nanoparticles. Chun-Wei Pao (RCAS, AS) has developed neural network methods for optimizing force field methods for any interested materials. Hsin Lin (IOP, AS) and Chi-Cheng Lee (TKU) have excellent experience in fitting the tight-binding model via the Wannier functions. For this research direction, physicists with excellent programming skills are crucial to this research direction. Extensive training in programming is needed. This research direction will couple with TG4.

Teams: Feng-Chuan Chuang (NSYSU), Ching-Ming Wei (IAMS, AS), Chun-Wei Pao (RCAS, AS), Hsin Lin (IOP, AS), and Chi-Cheng Lee (TKU).

(c) Recommendations on future critical hirings:

In this white paper, four important research directions have been identified, namely, (1) Two-dimensional Materials, (2) Topological Materials, (3) Correlated Materials, and (4) Machine Learning Guided Condensed Matter Research. Except for (3) Correlated materials, Taiwan already has strong teams to tackle these research directions. The training and education of young scholars can be enhanced through universities. The track of the research record of Taiwan-trained young scholars is already quite good. We will train our scholars well to succeed in the global competition. We recommend hiring Ph.D. graduates from Taiwan with sufficient international experiences, or foreign nationals with similar or better performance.

However, development of the calculations beyond DFT is still difficult for the current research groups in Taiwan. Thus, we will continue sending young scholars to pioneering groups to study these advanced methods. Also, we will advocate new hiring for scholars with expertise in *ab initio* strongly correlated methods, such as GW+DMFT and exchange-correlation functional development. In particular, candidates with the former expertise could synergize well with TG3.2.

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TG3.2 Strongly correlated condensed matter and cold atoms

Important directions in the next decade

(1) Correlation driven topological phases of matter and Majorana fermions

The discovery of symmetry protected topological insulators around 2005 has led to an enormous effort in trying to realize more exotic topological material phases both theoretically and experimentally, including: topological insulators, topological superconductors [3.2.1,3.2.2,3.2.3], Dirac and Weyl semimetals [3.2.4,3.2.5]. Spin-orbit couplings and specific symmetries of the systems play crucial roles in supporting these non-trivial topological and superconductivity properties. The most exciting phenomena of these topological materials are the gapless edge (surface) states protected by certain symmetries. Of particular interest are topological superconductors that support gapless self-conjugate, charge-neutral fermionic quasi-particle excitations. These excitations which reflect non-trivial topological bulk properties are localized at the edges, known as Majorana fermions (MFs) [3.2.1, 3.2.2]. Due to the robustness and non-Abelian statistics, MFs have been proposed to be an attractive candidate for realizing quantum bit (qbit) in building quantum computers. Much effort has been put in searching for signatures of Majorana fermions in solid-state materials. There have been possible signatures of MFs in metal-semiconductor wire hetero-structure. Extensive studies have been put to search for the topological states due to geometry or crystal symmetries in non-interacting or weakly interacting electron systems. More recently, interest has been shifted to search for topological phases and Majorana fermions induced by electron correlations [3.2.1]. The strong electron correlations may induce and stabilize the topological phases. We expect the correlation driven topological state of matter will be one of the most important topics in condensed matter in the coming decade.

(2) Novel quantum phases, quantum phase transitions in and out of equilibrium

In many-body condensed matter systems, strong electron correlations often lead to novel and exotic quantum ground states (or quantum phases), such as: Mott insulators, unconventional metallic and superconductivity in heavy-fermions and in cuprates, exotic spin-liquid phases in frustrated magnets.. Among them, the most challenging open problem is the understanding of the phase diagram of high-Tc cuprate superconductors, in particular the pseudogap phase at low hole doping of cuprates where many exotic phases have been discovered, such as: the charge-density-wave (CDW), spin-density-wave (SDW) and pair-density-wave (PDW) states . To identify these novel quantum phases is an important research direction in the coming decade.

Quantum phase transitions (QPTs) [3.2.6], the phase transitions at zero temperature due to quantum fluctuations, result in many fascinating but poorly understood phenomena in condensed matter and cold atom systems. Unconventional metallic or strange metal (SM) states are generic features in strongly correlated electron systems in equilibrium close to QPTs, including high-Tc cuprate, Fe-based superconductors, and heavy-fermion metals and superconductors. These "strange" phenomena in electronic and thermodynamic observables include T-linear or T-sub-linear power-law resistivity at low temperatures, a power-law singularity in spin susceptibility, a T-logarithmic specific heat coefficient. Due to the enhanced quantum fluctuations near quantum critical points (QCPs), a vanishing of the quasiparticle weight and divergence of the electron effective mass were observed. The quasiparticle picture within Landau's Fermi liquid (LFL) framework breaks down, hence the SM state is a non-Fermi liquid. The mechanism of strange metal has become one of the outstanding open problems in correlated electron systems. Previous theoretical attempts have not been successful to account for these exotic behaviors. A new paradigm is urgently needed to account for these phenomena [3.2.7,3.2.8]. Quantum phase transitions in superconducting nano-wire junctions are also actively studied in recent years [3.2.9, 3.2.10].

Due to the advances in experimental techniques, new surprising phenomena occur when systems close to out of equilibrium QPTs [3.2.11, 3.2.12] either by voltage bias (steady state non-equilibrium) or under a sudden quench (dynamical non-equilibrium). The former case can be realized in nano-devices (eg. a voltage biased quantum dot), while the latter has recently been realized in cold-atoms (Newton's cradle setup is realized in one-dimensional Bose gases) and nano-devices (pump-probe spectroscopy). Important fundamental questions to be addressed include: for steady-state QPTs--what is the different role played by the voltage bias near nonequilibrium QCP from that for temperature near equilibrium QCP? Is there a fluctuation-dissipation theorem similar to that in equilibrium? What is the distinct scaling form of observables from that in equilibrium? For quench QPTs--the time scales for thermalization, the possibility of pre-thermalized regime, quench dynamics near quantum phase transitions, and the existence of a generalized Gibbs ensemble (GGE) describing the steady state.

Besides, new interesting topics for many-body systems out of equilibrium arise when combining new theoretical approaches, such as: Evolution of entanglement spectra under generic quantum dynamics [3.2.13], Disorder-induced topology in quench dynamics [3.2.14].

(3) Fractionalization, quantum spin liquids, and emergent gauge theories

Fractionalization is one of the emergent quantum phenomena in strongly correlated systems. The most well-known case is the one dimensional Luttinger liquids, where the electrons are fractionalized into spinon and holon. In two dimensions, more exotic entanglement patterns could be realized and leads to fractionalized quasiparticles [3.2.15, 3.2.16,3.2.17], anyons, with non-trivial statistics. The study of such emergent phenomena is important for fundamental research and valuable for the developments of quantum technologies. One of the key ingredients to achieve such emergent quantum phenomena is the highly degenerated Hilbert space with non-trivial constraints. Frustrated quantum magnets are a suitable platform to study related phenomena since the competition in energy leads to macroscopic degenerate configuration with non-trivial local constraints [3.2.18]. Quantum fluctuations hybrid those degenerated states and lead to exotic fractionalization behavior. One important discovery for frustrated quantum magnets is the resonating valence bond (RVB) states proposed by P. W. Anderson in 1973. Any local order parameters vanish for the RVB state, suggesting such a quantum state of matter is beyond the Ginsburg-Landau paradigm. Such quantum states are highly entangled, to capture the non-local structure of entanglement, the low energy effective theory is closely related to the gauge theories. Besides, the gauge structure of the theory also provides non-trivial kinetic constraints and leads to novel dynamical behavior.

The fundamental questions in the topic are (1) How do the gauge fields emerge from the microscopic models that link to the effective gauge theories? (2) What are the properties of these fractionalized systems that can be experimentally probed and can be theoretically understood? (3) Are there other models that go beyond the current gauge theory description? (4) Physics of real-time dynamics of lattice gauge theories are poorly understood, how to design numerical methods to explore the possible interesting phenomena? (5) Bridging numerical methods and theoretical properties to identify highly-entangled quantum matter in experiments.

We will also try to use machine learning (or AI) techniques [3.2.19, 3.2.20] here to search for exotic quantum fractionalized spin liquid states in various quantum magnets.

Strength and opportunities for Taiwan

(a) Talents in Taiwan

The following researchers are talents in this field in Taiwan: The core members of TG3.2 (Chung-Hou Chung (NYCU), Sungkit Yip (Academia Sinica), Daw-Wei Wang (NTHU), Chien-Te Wu (NYCU), Shin-Ming Huang (NSYSU), Yi-Ping Huang (NTHU), Po-Yao Chang (NTHU), Shih-Yu Yu (NTNU)), Chung-Yu Mou (NTHU), Ting-Kuo Lee (NSYUS & IoP, Academia Sinica), Po-Chung Chen (NTHU), Ying-Jer Kao (NTU), Ming-Chiang Chung (NCHU), Jung-Jung Su (NYCU), Yu-Wen Lee (THU) Ming-Che Chang (NTNU), Sung-Po Chao (KNU), Baruch Rosenstein (NYCU), Hsien-Chung Kao (NTNU)

(b) Recommended strategy and teams to watch

We have the following achievements on the above topics in the recent years:

(1) Correlation driven topological phases of matter and Majorana fermions

We theoretically realized a novel fermionic finite-temperature Dirac points as critical points separating two topological phases in a Kondo lattice. It opens a new pathway to access the Dirac semimetallic phase and explore the fermionic critical point in the same system (PRL 2016). We proposed a new non-centrosymmetric superconductor on honeycomb lattice (pssb 2018, Editor's suggestion and cover image). We realized Dirac fermions and flat bands in the ideal kagome metal FeSn (Nature Materials 2020). We performed Full proximity treatment of topological superconductors in Josephson-junction architectures (PRB 2019). We established duality in topological superconductors and ferromagnetic topological insulators in a honeycomb lattice (PRB 2016). We review Noncentrosymmetric superconductors, (Annu. Rev. Condens. Matter Phys. 2014). We proposed a new helical Majorana fermions in $d_{x^2-y^2} + id_{xy}$-wave topological superconductivity of doped correlated quantum spin Hall insulators (Scientific Reports, 2016).We proposed a new geometry-induced topological superconductivity (PRB 2020).We demonstrated the duality in topological superconductors and ferromagnetic topological insulators in a honeycomb lattice. (PRB 2016). We realized quantum degenerate Majorana surface zero modes in two-dimensional space (PRA 2019). We calculated spontaneous thermal Hall conductance in superconductors with broken time-reversal symmetry (PRR 2020). We think our research performance so far along this line indicates that we are in state (B) and we have the potential to do well with sufficient support.

Recommended subjects:

-- Interplay of electron correlation and topological properties in topological insulators, e.g. topological Mott insulators, topological Kondo insulators, topological Weyl Kondo insulators.

-- Search for exotic surface superconductivity properties, e.g. Majorana zero mode on the surface of spherical topological insulator

-- Propose new topological superconductors mediated by Kondo interactions

--New approaches to realize Majorana fermions in correlated electron systems on novel 2D materials, such as: in graphene-based and Transition metal dichalcogenide (TMD) materials with honeycomb structures,

--Search for Majorana spin liquid state in Kitaev related spin models.

--Majorana fermions in Kondo insulators

Team: CH Chung, CT Wu, PY Chang, SM Huang, SK Yip, DW Wang, YP Huang

(2) Novel quantum phases, quantum phase transitions in and out of equilibrium:

We realized the PDW state in the t-J model via renormalized mean-field theory (Scientific Reports 2016). We proposed a new class of non-equilibrium quantum phase transition in quantum dot: Non-equilibrium transport at a dissipative quantum phase transition (PRL 2009, PRB 2013). We established a perfect agreement theory-experiment study in a non-equilibrium quantum critical steady state: Transport through a dissipative resonant level (PRR 2021). We realized theoretically a novel dynamical quantum phase transition in quantum link models (PRL 2019). We offer Quantitative studies of the critical regime near the superfluid-to-Mott-insulator transition (PRA 2017). We provided a mechanism for resolving outstanding open questions on strange metal and strange superconductivity in heavy-fermion Kondo lattices (PRB 2018, PRB 2019). We performed quantitative studies of the critical regime near the superfluid-to-Mott-insulator transition (PRA 2017). We proposed topological condensate in an interaction-induced gauge potential (PRA 2015). We studied the steady-state phase diagram of a weakly driven chiral-coupled atomic chain (PRR 2020). We developed a theory on topology and entanglement in quench dynamics (PRB 2018). We review Universal many-body response of heavy impurities coupled to a Fermi sea: a review of recent progress (Reports on Progress in Physics 2018). We think our research performance so far along this line indicates that we are in state (A): internationally competitive already.

Recommended subjects:

-Theory of pseudogap phase in cuprates as disordered PDW state (together with TK Lee))

--Mechanism of superconductivity in hydrogen superconductors

--Equilibrium and non-equilibrium topological quantum phase transitions

--Non-equilibrium and dynamical quantum phase transitions

--Mechanism of strange metal state in unconventional superconductors (cuprates, heavy-fermion, twisted bi-layer graphene)

--Quantum quench in light-matter interacting cold atoms, cavity quantum electrodynamics, quantum impurity, and low-dimensional interacting systems

--Quench dynamics at topological phase transitions

--Superconductivity with Tc above 85K was recently demonstrated in one unit cell FeSe on STO. Due to fabrication of one unit cell cuprate (BSCCO) layer without any suppression of superconductivity, the long standing problem of the theory of high Tc materials via Hubbard model description or the phonon mediated models have become part of the emerging 2D physics.(together with B. Rosenstein (NYCU) and Hsien - Chung Kao (NTNU))

Teams: CH Chung, PY Chang, DW Wang, CT Wu, JS You, YP Huang

(3) Fractionalization, quantum spin liquids, and emergent gauge theories

We developed a theory for disorder-free localization in 2D lattice gauge theory (PRL 2021). We studied quantum Kagome ice, theoretical study of the composite effect of space group symmetry, on-site symmetry and topological properties. (PRB 2017). We developed a theory on fractionalization in Kondo systems (PRL 2017). We had a theory on entanglement properties of the CS gauge theories (JHEP 2016). We think our research performance so far along this line indicates that we are in state (A): internationally competitive already.

Recommended subjects

---theoretical properties such as entanglement measures of the spin-liquids and other fractionalizations

--experimentally probes of the spin-liquids and other fractionalizations

---exact solvable models

---construct microscopic models that host non-abelian anyons and fractons

---dynamics and constrained systems

Team: YP Huang, CH Chung, CT Hseih, PY Chang

Recommended strategies:

The strategy to gradually form a team can be achieved by regular discussions and joint group meetings. Efficient ways of communications include: online seminar/meeting mixed with real meetings. We will host workshops/schools to provide interactions among members and training to students and postdocs. The strategies to move up to the frontier of this subject include: 1. to collaborate with the leading experimental groups worldwide (CCMS at NTU, NSRRC, TU Vienna, KIT Karlsruhe, Rice U., Kyoto U., Rutgers U., Max-Planck Institute, Dresden) to realize these proposed ideas and combine the experimental findings with theoretical predictions. These theory-experiment collaborative publications on novel topological superconductors are expected to show high impact. 2. to discuss and collaborate with the world leading theorists on these topics. 3. to participate in international conferences and to present our works there. 4. to invite world leading theorists and experimentalists on these topics to visit NCTS for a longer term to enhance the chance of collaboration.

Recommended hires:

We hope to recruit experts on the above topics (topic 1, 2, and 3) to strengthen our team.

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TG4: Interdisciplinary Research

TG4 is highly interdisciplinary, involving theoretical and computational research in strongly correlated many-body systems, statistical physics, atomic and molecular physics, chemical physics, biophysics, materials physics, soft matter physics, fluid physics, nonlinear physics, physical chemistry, physical biochemistry, and their interfaces (e.g., nanoscience, complex systems, and machine learning). We also study the interplay between machine learning and quantum physics and their deep connection.

Specifically, we develop and apply novel theoretical methods, such as tensor network method for classical and quantum systems, classical and quantum Monte Carlo methods, neural-network quantum states (such as restricted Boltzmann machine), quantum inspired algorithms for machine learning, quantum machine learning, quantum-mechanical (QM) methods (e.g., density functional theory (DFT), wave function theory (WFT), molecular mechanics (MM), statistical mechanics, molecular dynamics (MD) (e.g., classical MD, ab initio MD, and hybrid QM/MM MD), coarse-grained models, multiscale models, nonlinear dynamics, machine learning techniques, and many others, to predict and interpret physical, chemical, and biological phenomena occurring at different system sizes and timescales.

TG4.1: High-Performance Computation and Machine Learning

High-performance computation and machine learning are tools of increasing importance for many fields. Inspired by the concept of quantum entanglement, in the last decade tensor network method emerges not only as a novel numerical method to investigate strongly correlated but also as a new perspective for quantum matters. For example, it provides a natural language to describe symmetry protective and enriched topological phases. However, in order to tackle more complex systems in higher dimensions it is essential to design and implement the tensor network algorithms from the high-performance computation perspective. It is imperative to bridge modern high-performance computation (HPC) technology with tensor network methods. Here we feature a team applying these HPC tools to tensor network problems that have non-trivial connections to condensed matter physics, quantum field theory, quantum information and computation, and machine learning (see Fig. 6).

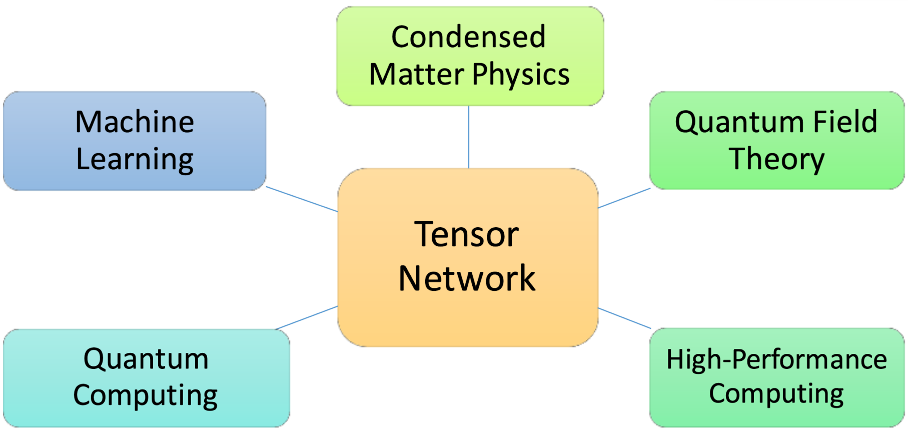

FIG. 6 Tensor network can be used as a tool to study fundamental problems in many different fields and their deep connections.

In the following we describe main objectives in more detail.

(1) Tensor network algorithms, libraries, and high-performance computation

In the last decade we have developed and applied algorithms based on tensor network states to study quantum many-body systems [4.1.1, 4.1.2]. In order to facilitate our research, we developed an open-source Universal Tensor Network Library (UNI10) [4.1.3], which is optimized for tensor network algorithms. The library provides high level APIs which can easily create and contract tensor networks with abelian symmetry, while the low level engines can be further optimized independently. We aim to develop new algorithms and methods for quantum many-body systems and big data analysis and to add support for non-abelian tensors [4.1.4]. We also aim to deploy the engines to a highly parallel, load-balanced distributed HPC environment, which requires expertise from applied mathematics, computer science, to quantum physics to solve the multifaceted problems in numerical linear algebra, process scheduling, and communication, and hardware optimization.

(2) Machine learning and quantum physics

Deep learning using artificial neural networks has in the past few years significantly changed many aspects of our everyday life [4.1.5, 4.1.6]. However, a broader understanding of why the current deep learning schemes work and novel algorithm proposals are highly coveted [4.1.7]. The connection between deep learning and physics has long been recognized [4.1.8]. Formalisms from quantum physics have been used to improve machine learning efficiency. Recently a mapping between a quantum many-body wavefunction in terms of a tensor network and in terms of a deep convolutional neural network is also established [4.1.9]. This points to a future direction of adopting tools in physicists' arsenal to understand and improve deep learning algorithms. Here the tensor network can serve as a bridge to explore ideas to exploit the potential of quantum computing to optimize classical machine learning algorithms.

(3) Tensor network, quantum information and computation

With the advances of quantum coherent control, quantum computers with hundreds of qubits seem to be on the horizon. Therefore, it is important to start thinking about what types of problems that can be solved in the immediate future using near-term quantum technology. These problems should be able to take advantage of quantum computing within a short coherent time and without full-fledged quantum error correction. The powerful graphical representation of the tensor networks has its origin from quantum circuits. The substantial theoretical understanding of the tensor networks in the classical setting can help us better understand and explore various aspects of quantum algorithms. Tensor networks also allow for algorithmic improvements in the classical setting readily transferred to the quantum setting. Tensor network circuits can be realized using quantum gates reachable by the near-term quantum computer, and they are a perfect tool to investigate this hybrid classical-quantum computing interplay. Recently, several schemes have been proposed linking ideas from tensor networks, quantum circuits, and machine learning [4.1.10, 4.1.11, 4.1.12], and this emerging field of interdisciplinary research has attracted great attention. Our experience in tensor networks, quantum algorithms, and software design places us in a strategic position to explore the near-term and future quantum computation.

A team called Taiwan Tensor Network Consortium has been formed including members of Ying-Jer Kao (NTU), Pochung Chen (NTHU), Chung Ming-Chiang (NCHU), Hong-Yi Chen (NTNU), Jhih-shih You (NTNU), Yu-Cheng Lin(NCCU), David Lin(NYCU), Po-Yao Chang (NTHU), Hsiu-Chuan Hsu (NCCU), Yi-Ping Huang (NTHU), Ching-Yu Huang (THU), Chia-Ming Chung (NSYSU) from physics and Che-Rong Lee(NTU), Wei-Chung Wang (NTU), Yen-Huan Li (NTU) from CS and Math.

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TG4.2a: Chemical Physics, Physical Chemistry, and Nanoscience

Important directions in the next decade:

With the vast advancement of computational hardware and software, the field of molecular simulations at various scales has grown tremendously in the past decades. The quantum mechanics for the electrons in molecules, and the dynamics at various levels of coarse-graining at a larger scale, can be routinely solved or simulated for standard problems with reasonable precision. Computer simulation in chemical physics, physical chemistry, and nanoscience (i.e., molecular sciences) have become much more feasible. As a consequence, molecular simulation and computation have been a nearly indispensable ingredient in modern, edge-cutting research. Therefore, it is important to develop fundamental theories related to molecular simulation and computation, and to extend the boundaries of feasible or understandable problems. Notable new developments include (a) those that improve the computational costs as well those lift limitations imposed by the approximations employed in the current theories or algorithms, (b) theoretical developments that can cope with the complexity of the realistic situation seen in both experiments and in computer simulation, and, (c) application/computational works that could either offer further insights, or extend the scope of experiments.

Specifically, these important areas can be laid out as follows.

(1) **New theoretical advancements that could improve the computational costs and lift limitations imposed by the approximations employed in the current theories or algorithms**

(i) *Treatment of static correlation in density functional theory (DFT):* As a single-determinant based theory, the Kohn-Sham DFT [4.2a.1] has been computationally feasible, and convenient to develop. However, the singlet-determinant nature has also been an obstacle in treating systems with strong static correlation [4.2a.2]. Much effort has been devoted in this area, and an approach that provides accurate results while maintaining the level of computational complexity is yet to be developed [4.2a.3~4.2a.12].

(ii) *Static correlation for chemistry problems:* With several promising approaches currently available in the popular computational chemistry programs, it is important to address the chemistry problems with static correlations included. Specifically, a ground-state method with static correlation could enhance the description of bond-breaking and formation, as well as the charge-transfer situation. Methods with excited state capacities could be used to study photochemistry with good faith, as well as various excitation energy transfer and/or excited state charge transfer problems [4.2a.11,4.2a.13~4.2a.15].

(2) **Theoretical developments that can cope with the complexity of the realistic situation seen both in experiments and in computer simulation**

(i) *Large-scale coherence dynamics of molecules:* Coherence plays a significant role in chemistry, and it is associated with the design of organic devices (OLED or solar cell), the mechanism of photosynthesis, and quantum electrodynamical chemistry [4.2a.16,4.2a.17]. However, traditional methods cannot cope with the complexity of realistic situations well. As a result, it is necessary to develop new theoretical approaches which combine open quantum system techniques and first-principle calculations together [4.2a.18~4.2a.20].

(ii) *Unified theoretical understanding with simulated spectral density:* The mechanism of decoherence in molecules is one of the most important topics in chemistry (e.g., photoinduced electron transfer, nuclear magnetic resonance, spontaneous emission, molecular electronics, resonance energy transfer), and it is related to the structure of spectral density. Vibronic coupling and light-matter interactions can induce or suppress the decoherence of molecules, and how to obtain the spectral density from molecular vibrations or photonic environments is a key issue to understand the mechanism of decoherence [4.2a.21].

(iii) *Multi-scale simulations:* Multi-scale simulations allow us to connect microscopic molecular descriptions to macroscopic properties and problems, which are essentially important in nanoscience and soft materials such as polymers. The intermolecular (inter-particle) interactions and structural configurations of the materials play an important role in the appearance of macroscopic properties [4.2a.22]. Thus, the development of molecular mechanical force fields, including physics-based and knowledge-based approaches, has been an important area. A proper coarse-grained modeling method would allow simulation for very large systems without having to pay a large amount of computational cost [4.2a.23,4.2a.24]. Machine learning-based forcefields could also allow the large-scale simulation of complex material systems such as high entropy materials or complex perovskites with high fidelity with first-principle calculations [4.2a.25~4.2a.27]. Simulations employing multi-scale models in conjunction with efficient sampling techniques of configuration space could also decipher the complex mechanisms of cell membrane insertion of bio-macromolecules, more significantly, the COVID-19 infection. The methodologies in the sampling techniques, and in the analyses, are also of fundamental importance. Effective sampling methods allow researchers to observe important and yet rarely seen events in the simulation. Due to the large size and the huge number of degrees of freedom such works typically are with, extracting useful information with advanced theories and methods is essential. Redox reactions under applied voltages are examples of chemical reactions under external environments. Application of external voltage to an electrode can readily modulate the structure of the electrode-electrolyte interface, providing an external driving force to affect chemical processes such as catalytic reactions. As many redox reactions occur at the interface between the solid electrode and liquid (electrolyte) solutions, the chemical processes at electrochemical interfaces should be investigated with the full influence of electrode, solution composition, and external voltage. However, the modulation due to the physical structure of the electrode-electrolyte interface is explicitly neglected in quantum mechanics studies [4.2a.28~4.2a.30]. A computational/theoretical modeling thus requires methods for the first principle description of the electrode-electrolyte interactions at a fixed potential, including how to incorporate applied voltage and electrode-electrolyte interactions into force field parameters in ab-initio fashion, how to efficiently sample the probability distribution of redox states, how to capture the charge flow to/from the electrode. As the dynamical evolutions of electrolyte composition, interfacial structures and interactions, and redox states are strongly modulated by external voltage [4.2a.31~4.2a.34], computational characterization approaches for the response of electrochemical interfaces will be important for harnessing voltage to control desired chemical application.

(3) **Application/computational works that could offer further insights, or extend the scope of experiments in chemistry and physics.**

(i) *Spectroscopy analyses and prediction of spectral features of functional materials:* The prediction or determination of the relationship between the geometrical feature of functional materials and their spectroscopy features are needed for experimentalists to gain further physical and chemical insights of the functionalities. First principle spectroscopy simulations mainly based on the energy domain may serve this purpose by targeting the electronic excitation spectroscopy (valence/core electrons) [4.2a.35~4.2a.37] and the absorption and/or scattering spectroscopy of the phonons/vibrations [4.2a.38~4.2a.53].

(ii) *The chemical reaction at/on catalytic active surfaces and compounds:* Many chemical processes are carried out via catalytic reactions. However, for many systems, the catalytic active species and/or the catalytic active sites have remained an open question [4.2a.54]. To understand and design a catalytic process based on theoretical considerations, it is required to have information on the nature of the "frontier orbitals": information related to the phase symmetries and energies of the wave functions of the chemically important orbitals for the reactant and catalyst [4.2a.55~4.2a.63]. The investigation of those properties can, for instance, be applied to semiconducting 2D materials, a novel class of catalytic materials that can be easily functionalized chemically or physically by introducing "defects" during the material synthesis. The application of light to such materials may lead to the formation of defective areas on the surfaces of such materials, which may be important for the catalytic activity. The existence of such sites on 2D materials is well-accepted by many experimental groups; theoretical investigations can help to clarify their exact role in catalytic processes. The grand target of this topic is to understand catalytic processes sufficiently well in order to provide experimentalists with a guiding principle of choosing reactants, products, and catalyst/catalyst modifications to achieve a desired reaction. Reactions of interest include, for example, the activation of H_2, O_2, H_2O, or CO_2, over defective 2D metal oxides and defective 2D transition metal chalcogenides [4.2a.64] as well as other (homogeneous and heterogeneous) catalysts.

(iii) *Degrees of freedom of the spin, orbital, and charge of molecules under external environments (strongly correlated electrons and quantum chemistry):* Among transition metal oxides compounds, there exist the so-called strongly correlated electron systems. Recently, chemical reactions with such strongly correlated systems have drawn attention, for example, 4 Mn ions in the water splitting site of natural photosynthetic systems [4.2a.65~4.2a.68] and the decomposition problem of spinel $LiNi_{0.5}Mn_{0.5}O_4$ in electrolyte for high-voltage lithium-ion batteries [4.2a.69]. The elucidation of the relationship among the structure, orbitals, charge state, and spin state is the first step to understand chemical reactions of strongly correlated electron systems. First principle simulation approaches may shed light on how these three properties are entangled in chemical reactions of strongly correlated systems [4.2a.70]. This topic may promote the opportunity of having an interaction with condensed matter physicists.

(iv) *Electronic structure of new materials (crystalline)*

Metal-organic frameworks (MOFs) have become popular materials because these sit at the interface between molecule and material. Owing to diversity in their structures and composites, various allocation usages ranging from catalysts to electrical conductors, photo-induced chemical transformations and more have been proposed. DFT simulations for electronic structure determination can provide useful information on the electronic properties that may arise from these frameworks [4.2a.71]. MOFs can serve as a challenging stage for the quantum chemists to explore electronic structure theory to deal with reactivity and electron transfer using periodic, molecular and embedded models.

Strengths and opportunities for Taiwan:

For the scientific topic (1), in recent years, a large amount of advances has been made in the development of Kohn-Sham density functional theory (KS-DFT) [4.2a.1] for novel exchange-correlation energy functionals for much improved computational performance. Among all the problems with current KS-DFT, the static correlation (SC) (also called strong correlation or non-dynamical correlation) problem is perhaps the most prevalent and hardest to resolve [4.2a.2,4.2a.3]. In wavefunction based theories, SC is a correlation effect that can be handled by including nearly degenerate configurations. Various approaches aiming to resolve the SC problem are emerging in recent years. Traditional treatment of SC requires a full configuration interaction (FCI) in the active space, resulting in expensive computation and it often requires trial-and-error in the setting. Therefore, tackling SC with alternative means, especially those without FCI in an active space, is highly desirable. Jeng-Da Chai's (NTU) thermally-assisted-occupation density functional theory (TAO-DFT) [4.2a.4~4.2a.6] has been one of such highly desirable developments, for treating SC with easy setting and small additional computational costs. Owing to its computational efficiency, TAO-DFT has been recently applied to explore the ground-state properties of various electronic systems at the nanoscale, especially for those with pronounced SC [4.2a.8~4.2a.10]. Very recently, TAO-DFT has been combined with ab initio MD to explore the dynamical information of nanosystems with pronounced SC at finite temperatures [4.2a.12]. Along a similar line, Chao-Ping Hsu has started employing the Restricted Active Space (RAS) approach developed by Martin Head-Gordon and coworkers and elaborate its application in charge and energy transfer processes [4.2a.13,4.2a.14].

For the topics (i) and (ii) in (2), Jer-Lai Kuo (AS), Chao-Ping Hsu (AS), Liang-Yan Hsu (AS), Michitoshi Hayashi (NTU), Yuan-Chung Cheng (NTU) and Bih-Yaw Jin (NTU) are outstanding experts in these subjects in Taiwan. For example, Jer-Lai Kuo has developed a very powerful method to include anharmonic effects in molecular spectra. The method developed by Chao-Ping Hsu can be used to study exciton diffusion and energy transfer at the first principles level. Liang-Yan Hsu has recently established a general theory of resonance energy transfer and molecular fluorescence based on macroscopic quantum electrodynamics. Michitoshi Hayashi focuses on the development of theories and calculations of the THz spectra of molecular crystals. Yuan-Chung Cheng is an expert in open quantum systems and non-adiabatic dynamics, and applied these techniques in photosynthesis. Bih-Yaw Jin focuses on establishing the theories of organic electronics and optoelectronics based on semi-empirical methods. Currently, Carmay Lim (AS), Lee-Wei Yang (NTHU), Jhyh-Wei Chu (NYCU), Jung-Hsin Lin (AS), Jer-Lai Kuo (AS), Chun-Wei Pao (AS), and Yi-Jung Tu (NCNU) are outstanding PIs in topic (iii). The support of NCTS will be used to promote cross (sub-)disciplinary discussions and collaborations for the best research influences and outcome.

There are several quite prominent PIs for the topics in (3), notably Jyh-Chiang Jiang from NTUST, Chin-Hui Yu from NTHU, Jen-Shiang Yu from NYCU, Michitoshi Hayashi and Yi-Pei Li from NTU, Ming-Kang Tsai from NTNU, Kaito Takahashi from AS, and Cheng-chau Chiu from NSYSU. Overall, this is the major strength of Taiwanese computational physical chemistry community. In the past, Jyh-Chiang Jiang has successfully predicted an important advantage of IrO_2 in the activation of C-H bond, a class of important chemical reaction that's once called "the holy grail" for its huge impact on the industry and its intrinsic difficulty. Biological chemistry, including enzyme-facilitated and biomass utilization, has also been studied (Chin-Hui Yu and Jen-Shiang Yu). Besides, the dual-defective SnS_2 monolayer has been predicted to be an efficient photocatalyst for overall water splitting to generate hydrogen fuel (Michitoshi Hayashi). Recently, works on the chemical feature space and the target machine-learning have also been developed (Yi-Pei Li). Various inorganic reactions, as well as reactions on surfaces were also studied. For the very basic aspect of chemical reaction, a quantum chemistry simulation accuracy of a chemical reaction rate constant has been discussed thoroughly (Kaito Takahashi). For the First principle spectroscopy simulation topics, Jer-Lai Kuo (AS) who works on vibrational spectral features due to anharmonicity of molecules, Po-Tuan Chen (NTUT) who is an expert in first principle simulations on core electron spectroscopy and Michitoshi Hayashi may make some contributions.

Recommended strategy:

1. A jointly hired postdoc: Formulation of theory, coding, and real scientific issues that are interconnected. Thus exchange of knowledge among the research areas (a)~(c) is necessary and would largely facilitate the pace of research progress and understanding of the problems. Specific knowledge on computational simulations (coding, installation and optimization of packages and libraries, and/or experiences in usage or packages) may be appreciated by large populations of the community.
2. TG4.2a may host study groups to promote collaborations among domestic theoretical/computational research groups. The study topics may be related to new theoretical developments, theoretical tools, etc. Each study group may be initiated by any core members in TG4.2a.

Recommendations on future critical hirings:

1. While NCTS cannot directly appoint permanent researchers, our identification of important future directions could help the community in various peer-reviewing research proposals and in the recruitment process of their home departments.
2. To cultivate young researchers in Taiwan, TG4.2a shall hold relevant activities (e.g., regular

meetings, annual workshops, international conferences, supporting visiting researchers). Besides, we plan to work closely with Taiwan Theoretical and Computational Molecular Science Association (T2CoMSA), making successive efforts in educating students and promoting young researchers in theoretical and computational chemical physics, physical chemistry, and nanoscience.

3. The postdoc position under TG4.2a should be regarded as prestigious in the theoretical and computational chemistry community domestically and, ideally, internationally. It may serve as a tentative position of a person with an excellent research performance ready for an academic position in Taiwan.

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TG4.2b Complex Systems

Important directions in the next decade:

The physics of Complex Systems (CS) typically covers a wide range of interdisciplinary topics. For the Taiwan physics community, the CS thematic group has served the physics communities of non-linear statistical physics, granular and molecular complex fluids, biological physics, soft matter physics, and network physics. In the past two decades, these fields have seen tremendous growth globally. *The American Physical Society has four separate Divisions in Polymer Physics, Fluid Dynamics, Soft Matter, Biological Physics, in addition to the Topical Group on Statistical and Nonlinear Physics. The Biophysical Society and the Division of Fluid Dynamics have separate annual meetings, each with attendance of over 2000 members.*

As more advanced and high-resolution physics tools become available to study complex systems on the molecular scale, there has never been a more exciting time to work on physics in these fields on problems such as the physical properties of DNA, proteins, and the mechanisms of gene translation. How metastasized cancer cells are transported via the bloodstream, and how micro-devices could employ fluid physics for finding one cancer cell in a billion blood cells. How self-propelling micro-particles such as bacteria swarm like schools of fishes to swim faster collectively. How network structure and connectivity determine information transfer between protein molecules for cells to function and between cells for organisms to live and evolve.

The science in these fields has also been more recognized as having made impactful contributions. Nobel prizes in chemistry were given in 2011 for the discovery of quasi-crystals, in 2014 for super-resolution microscopy, in 2017 for cryo-EM development for studying biomolecules, in 2018 for directed evolution that nowadays extend into statistical physics and network physics of proteins, in 2020 for CRISPR that developed an epoch-making and powerful genetic editing technique from a bacterial evolutionary immune mechanism, and in physics for the development of the optical tweezer and its application for studying biomolecules.

Although the local physics community in these areas is small, we actively organize regular workshops aimed at training junior scientists, establishing domestic collaborations within and outside the physics community, and invite international experts to visit, to network, and to exchange frontier developments in these areas. A nexus for nurturing junior scientists has formed at National Central University, National Tsing-Hua University, and Academia Sinica. There have been many successful recent trainees. Amongst many, Wen-Tau Juan (NCU, Stanford, Chinese Medical U.), trained in plasma, polymer, and fluid physics, recently used his expertise to study the physical properties of bird feathers, which was published in Cell. Hong-Yan Shih (NTHU, UIUC, AS, APS GSNP Dissertation Awardee), trained in statistical and condensed matter physics, developed a new paradigm for studying transitional turbulence using non-equilibrium statistical mechanics and biological models, now investigating emergent spatiotemporal patterns in fluid turbulence and biological systems.

Following NCTS's existing mission to develop and encourage collaborations and nurture junior scientists, the Complex Systems Thematic Group has supported research activities that strengthen communication and collaboration in interdisciplinary Complex Systems studies. The major Research Themes are

- Physics of complex networks and pattern formation
- Physics of field induced structural organization in soft matter and complex fluids
- Emergence of self-organization in active, self-driven particles and organisms
- Stochastic thermodynamics and information physics

Strengths and opportunities for Taiwan:

The general philosophy in the Complex Systems Physics is to reduce complexity to simplicity – similar to cellular automata, to reproduce complex behavior with simple rules. In the event that the complexity is too great, such as in weather prediction, stock market movement, fluid turbulence, one seeks to find physical characteristics that are analogous to other simpler systems, such as found for critical phenomena and universality classes. In recent years, several hot topics have emerged, including (1) collective motion of active particles, such as found for bacteria swarming, synchronized protein oscillations, and fish schools. (2) Mapping of turbulent flow to predator-prey universality class. (3) How mechanical deformations affect cell and cell cluster dynamics under flow and in constricted environments.

(a) Talents in Taiwan:

Hsuan-Yi Chen (NCU), Pik-Yin Lai (NCU), Chien-Jung Lo (NCU), Cheng-Hung Chang (NYCU), Kuo-An Wu (NTHU), Lee-Wei Yang (NTHU), Hong-Yan Shih (AS), Yeng-Long Chen (AS), and Sheng-hong Chen (AS)

Within Taiwan, and particularly in this TG, active collaborations are tackling several of these problems.

- Kuo-An Wu (NTHU) is currently focusing on mechanisms of pattern formations in complex systems such as biophysics and materials science. KAW collaborates with Gururajan Mogadalai (IIT, Bombay) on the morphology of microstructural evolution which requires fundamental understandings of interfaces in materials across the various length and time scales. KAW and HYC (Hsuan-Yi Chen, NCU) collaborate with Shigeyuki Komura at Tokyo Metropolitan University to investigate pattern formation of skin cancers and examine the hydrodynamic effects on pattern formation [4.2b.1]. KAW also works on reduced dynamics of a cardiac cell with Daisuke Sato at UC Davis that would shed light on the mechanism of cardiac alternans which is closely related to several cardiac diseases.

- Yeng-Long Chen (AS) is collaborating with the Non-Newtonian Fluid Mechanics Group at MIT to develop a physics-based model to understand the hierarchical structure and the time-dependent response of particle-laden complex fluids with polymer solutions, micro-particles, and biological cells. On-going collaborations include modeling how major cardiovascular surgery affects patient blood viscoelasticity with the Tri-Services General Hospital [4.2b.2], and to understanding how metastatic tumor cell clusters transport across the blood vessel [4.2b.3].

- Cheng-Hung Chang (NYCU) proposed a chemical potential formalism for polymer entropic forces [4.2b.4] and derived formulae for recoiling, tension, and drift entropic forces for polymers partly confined in 2D strips, 3D tubes, and 3D slits, with both hard and soft boundaries. It confirms and clarifies several recent granular and polymer experiments, including the confined granular chains on a vibrating platform [Kiwing To (AS) and Ya-Chang Chou's groups at Phys. NTHU] and DNA recoiling and tug-of-war in nanochannels, nanopillar arrays, and nanoslits [Yeng-Long Chen and Chia-Fu Chou's groups at Academia Sinica].

- Hong-Yan Shih (AS) and her thesis advisor Nigel Goldenfeld (UIUC) have developed a new paradigm for transitional turbulence using statistical mechanics and discovered its surprising connection to biology, renormalization group theory and high-energy hardron scattering. HYS is now collaborating with experimentalists and theorists in the U.S. and Europe to generalize the framework to universal critical behavior in turbulence and the emergent evolutionary patterns in bacteria-virus and immune systems.

- Sheng-hong Chen's (AS) group is focused on investigating two fundamental questions in biological complex systems. The first is how biological dynamics emerge from collective behavior of signaling molecules in single cells. His group quantifies dynamics of signaling molecules in single cells and analyzes systems behavior *in silico* using mathematical and statistical modelings. The second is how cellular patterns emerge from collective behavior of individual cells and their biological significance during stress responses. The overall goal is to understand systems properties of human cells in order to control cellular decisions for therapeutic purposes.

- Lee-Wei Yang's group leveraged their molecular dynamics expertise in partnership with Academician Ming-Daw Tsai's (AS) group, housing the state-of-the-art cryo-EM technique, to resolve 5 ribosome structures at atomic resolution (~3A), each of which in rotated, non-rotated or rotated-and-rolled state in the presence or absence of a frameshifting-triggered RNA pseudoknot at the 30S entrance. The ribosome particles are prepared by long-term collaborator Jin-Der Wen in NTU. Lee-Wei Yang's group in NTHU validated their earlier predictions on these conformational transitions and explained the mechanical causes of the transitions in the presence of RNA pseudoknots [4.2b.5] using a DGX A100-accelerated GPU-based simulator to achieve ~25 ns/day for a fully solvated ribosome comprising more than 2.5 million atoms.

In addition to the above highlighted theoretical and computational research, there have also been leading experimental research in plasma physics (I Lin and collaborators, NCU) and physical neuroscience (Ann-Shyn Chiang, NTHU), with many opportunities to be pursued.

(b) Recommended strategy and teams to watch:

Statistical physics, network sciences, fluid physics, and biophysics played important roles in understanding the Sars-Cov-2 virus and paths of transmission during the Covid-19 pandemic. This cross-disciplinary intersection between physics and biology will grow significantly more important in the coming decade. With simultaneous advances in experimental capability to see single molecules and measure various properties of cells, we expect accelerated advancements in theoretical and computational soft matter and biological physics for problems ranging from molecules to cells to large organisms.

In particular, the following topics are at the intersection of research frontiers in the upcoming decade:

- Atomic resolution imaging and advanced computation

With advances in GPU-accelerated simulations, cryo-electron tomography, and single molecule imaging, it starts to become possible to resolve macromolecules of tens or hundreds of megadalton to the atomic level and simulate the dynamic interactions between them. In the next decade such (resolution-exchange) simulations with the corresponding theoretical development on efficient sampling methods and free energy calculations could be extended and carried out in the context of a living cell or a viral particle at a meaningful time scale (from sub-seconds to minutes) [4.2b.6] in an all-atom or coarse-grained presentation to study phase-phase separation, autophagosome formation, protein or mRNA translocation through pores, ribosome translation [4.2b.5-4.2b8], bacteria flagella growth (or motor rotation) at real time [4.2b.9,4.2b.10]. (Lee-Wei Yang, Chien-Jung Lo, Cheng-Hung Chang)

- Inter-cell communications, inter-particle interactions, network formation, and self-organization

Advances in real-time simultaneous tracking of the trajectories of numerous microparticles and cells have enabled discoveries of self-organized collective behavior of active living [4.2b.11,4.2b.12] (cells, viruses) and non-living systems (polymers, Janus particles) [4.2b.13, 4.2b.14], and new analogies are made between the polarized ordering of cells to the aligned nematic order in liquid crystals and stiff polymers [4.2b.15]. In addition, discoveries of exosomes -- nano-vesicles produced by cells -- could solve key mysteries on how cells communicate with each other.

We expect that in the coming decade, significant progress could be made in understanding how cells self-organize by understanding the physical principles that govern collective dynamics and phase behavior of non-living active macromolecules. Furthermore, new discoveries of how cells communicate and interact with each other could be imitated in model non-living but active microparticle systems, with significant opportunities for physical sciences to develop new insights into the principles that guide living systems. New machine learning, theoretical, and computational technologies will help to identify characteristics that could be further investigated to understand the mechanism, the advantages, and the consequences of self-organized behavior. In collaboration with experiments, we may progress to understand how particle motility drives living organisms. (Sheng-hong Chen, Yeng-Long Chen, Hsuan-Yi Chen, Kuo-An Wu, Hong-Yan Shih, Pik-Yin Lai)

(c) Recommendations on future critical hirings:

Although Complex Systems has increasing visibility in physical sciences, truly cross-disciplinary collaborations and training need strong communication between physicists, chemists, biologists, and engineers. The on-going trend, and the trend for the next decade, will see more interdisciplinary research to understand the physics of biological organisms, particularly epidemic-related topics such as viral transmission, viral assembly, and viral replication. Physics will also become significantly more involved in areas such as cell and molecular manipulation and control, for applications such as cell separation, microparticle drug delivery, fluid manipulation, and nano-engineering. These research areas require physicists to broaden their training in statistics, biology, chemistry, fluid mechanics and engineering. To help developing junior scientists in these areas, we recommend

- *Creation of Training Postdoctoral Fellowships, with two to three year terms, to encourage junior scientists to join cross-disciplinary research, during which they will have time to learn new skill sets.*

- *Creation of interdisciplinary research positions, providing additional incentives -- salary and research funding -- for cross-departmental and cross-institute hirings.*

- *Encourage long term research + application partnerships that provide opportunities for advanced graduate students to direct their projects towards future applications, with incentives for increased stipend and career outlooks.*

Furthermore, although cross disciplinary physics research in statistical physics, fluid dynamics, soft matter, and biological physics have increased presence globally, its growth in Taiwan has been stagnant. Many leading physics departments have less than 10% representation of faculty in these areas. With a global highlight on the pandemic crisis in addition to the climate change crisis, these fields are most relevant within the physics community to understanding these problems with the potential of finding solutions. *Taiwan could and should significantly invest in cluster hiring of physicists trained in biological physics, fluid physics, and statistical physics, with the goal of raising the representation in the Taiwan physics community to at least 15 % and aim for 25 to 30 % by 2040.*

One big challenge that many fields face is how to recruit high quality new research scientists. Besides some obvious issues such as compensation reform that neighboring states have taken (South Korea, Singapore, Hong Kong, PRC), some success cases are to hire well-known and respected international scientists to start focus centers within universities. South Korea's IBS Center for Soft and Living Matter, led by Steve Granick, is a success model that involves domestic scientists along with new international hires. These projects could raise international visibility and credibility and help with recruitment by learning from neighboring states' experiences on what works and what doesn't.

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