Strange diffusion constant of incoherent metal in half-filled two-dimensional Hubbard model

Youngmin Eom[1], Igor S. Tupitsyn[2], Nikolay V. Prokof'ev[2], Boris Svistunov[2], Evgeny Kozik[3], and Aaram J. Kim[1]*

[1]Department of Physics and Chemistry, DGIST, Daegu 42988, Korea
[2]Department of Physics, University of Massachusetts, Amherst, Massachusetts 01003, USA
[3]Department of Physics, Kings College London, Strand, London WC2R 2LS, United Kingdom
Email*: aaram@dgist.ac.kr

We study the incoherent charge transport in the prototypical half-filled two-dimensional Hubbard model from the viewpoint of the Nernst–Einstein relation. Using the numerically exact diagrammatic Monte Carlo method, we calculate the dynamic current–current correlation function in the thermodynamic limit and perform the analytic continuation for the optical conductivity using the stochastic optimization method. Our analysis reveals an unconventional $1/\sqrt{T}$ dependence of the diffusion constant over a wide range of temperatures and interaction strength, where the DC resistivity exhibits anomalous T or $\sqrt{T}$ scaling. This behavior is intriguingly consistent with the recent results of ultracold atom experiments on doped systems [1]. Furthermore, by distinguishing the bubble and vertex diagrams in the optical conductivity, we demonstrate that the bubble term is the main source of incoherent transport in high temperatures while the vertex correction becomes significant only near the metal-to-insulator crossover regime.

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Fictitious Temperature in TAO-DFT

Jeng-Da Chai

Department of Physics, National Taiwan University, Taipei 10617, Taiwan
Physics Division, National Center for Theoretical Sciences, Taipei 10617, Taiwan
Email: jdchai@phys.ntu.edu.tw

In contrast to the widely used Kohn-Sham density functional theory (KS-DFT), thermally-assisted-occupation density functional theory (TAO-DFT) [J.-D. Chai, J. Chem. Phys. 136, 154104 (2012)] is a density functional theory with fractional orbital occupations given by the Fermi-Dirac distribution (controlled by a fictitious temperature), for the study of large electronic systems with multi-reference character. Owing to its computational efficiency and reasonable accuracy, TAO-DFT has been recently applied to the study of various nanomaterials with multi-reference character (i.e., challenging systems for conventional electronic structure methods). The role of TAO-DFT fictitious temperature and a few interesting results will be presented.

Theoretical study of excitonic effects in semiconductor moiré materials

Yao-Wen Chang

Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 106, Taiwan

In the first part of this talk, a continuum model for the theoretical study of hybridized moiré excitons in transition metal dichalcogenides heterobilayers will be introduced. The exciton continuum model is built by the charge continuum model for electrons and holes in moiré superlattices, thereby preserving the moiré periodicity and lattice symmetry from the charge continuum model. The momentum-space shift of interlayer electron-hole distribution is included, and thus the indirect nature of interlayer excitons is described. The spin and valley degrees of freedom and related interactions are omitted, except for the spin-orbit energy splitting of A and B excitons. This continuum model is applied to the simulation of optical absorption by hybridized moiré excitons in WSe_2/WS_2 and $MoSe_2/WS_2$ heterobilayers. Simulations of twist-angle and electric-field dependences of optical absorption spectra will be shown and discussed. In the second part of the talk, the concept and application of interlayer-exciton condensation in moiré mateirals will be introduced. An exciton is composed of two fermions and can be viewed as a composite boson. It was predicted that, below a critical temperature, an exciton gas could undergo a transition to form an excitonic Bose-Einstein condensate, resulting in the electronic system becoming an insulator known as the exciton insulator. With an additional moiré degree of freedom, exciton condensates in 2D layered materials becomes even more intricate. Moiré-exciton condensates exhibit incompressibility, indicating that the condensate represents a bosonic correlated insulator of excitons. The behavior of this bosonic correlated insulator can be described using a Bose-Hubbard model. The magnetic and transport properties of moiré-exciton condensates may be influenced by their strongly correlated nature.

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Investigation of light-matter interaction through time-dependent density functional theory: microscopic mechanism of photocurrent generation

Jeongwoo Kim

Department of Physics, Incheon National University, Incheon 22012, Korea
Email: kjwlou@inu.ac.kr

Light-matter interaction has been investigated through the estimation of response functions derived from perturbation theory, leading to a successful understanding of intriguing quantum phenomena. While perturbation theory has provided valuable insights into light-matter interactions, fully capturing the temporal dynamics of electrons and the lattice, particularly under strong external fields, remains a challenge. In this presentation, I will discuss the behavior of electrons subjected to external electric fields of varying strengths using time-dependent density functional theory (TDDFT), an increasingly important method for understanding the complex interplay between electrons and lattice. Specifically, the underlying mechanism of giant shift currents in non-centrosymmetric low-dimensional systems will be presented. It has been found that the giant shift currents in WS_2 and Bi nanotubes [1,2] originate from interchain interactions and a nontrivial electronic structure, respectively. The presence of orbital angular momentum induced by an external field in helical materials, and its optoelectronic manifestations, will be discussed.

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Excitonic effects on Raman, infrared absorption spectroscopy, and coherent phonon from ab initio time-dependent aGW approach

Yang-hao Chan

Institute of Atomic and Molecular Sciences, Academia Sinica
Physics Division, National Center for Theoretical Sciences
Email: yanghao@gate.sinica.edu.tw

The interplay between electron-phonon couplings and electron-hole correlation effects in electron dynamics is fundamentally interesting and relevant for applications ranging from energy harvesting to quantum information sciences. We extend the time-dependent adiabatic GW (TD-aGW) theory to include electron-phonon (e-ph) couplings with a classical phonon approximation. Based on a perturbative expansion of electron-phonon and electron-light (e-l) couplings, we derive the infrared (IR) absorption and Raman scattering spectra with excitonic effects. We show that excitonic effects can be included by dressing the proper e-ph or e-l vertices with electron-hole ladder diagrams, which are readily available from standard GW-Bethe-Salpeter equation calculations. We demonstrate that the exciton-phonon coupling strength and exciton energy landscape can be accessed by analyzing resonance Raman spectrum. We further explore coherent phonon signatures in time-resolved angle-resolved photoemission spectroscopy for a monolayer MoS2 by conducting real-time simulations with the developed approach.

The work was done in collaboration with Zhenglu Li from University of Southern California (USC) and Prof. Steven G. Louie from University of California, Berkeley. Work done in UC Berkeley and USC was supported by the Center for Computational Study of Excited State Phenomena in Energy Materials (C2SEPEM), which is funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract No. DE-AC02-05CH11231. YHC acknowledges support by National Science and Technology Council and National Center for High-performance Computing (NCHC) for providing computational and storage resources in Taiwan.

Next-Nearest-Neighbor Coupling Effects on Thermodynamics of the Spin-1/2 Hyperkagome Lattice

Ara Go

Department of Physics, Chonnam National University, Gwangju Republic of Korea
Email: arago@jnu.ac.kr

We present a theoretical investigation of a spin-$\frac{1}{2}$ hyperkagome lattice described by a $J_1 - J_2 - D$ Hamiltonian, where J_1 and J_2 are the nearest- and next-nearest-neighbor antiferromagnetic exchange couplings, respectively, and D is the dipole–dipole interaction. Using exact diagonalization and thermal pure quantum calculations, we explore the low-temperature thermodynamics of this highly frustrated system. Our results indicate that the next-nearest-neighbor coupling J_2 plays a pivotal role in modulating both the specific heat capacity and the degeneracy structure of the lowest-energy eigenstates. In particular, the inclusion of J_2 leads to a marked change in the peak structure of the specific heat, suggesting a possible crossover or phase transition regime at low temperatures. We compare these theoretical findings with experimental heat-capacity measurements on Yb-based hyperkagome compounds, enabling us to propose a plausible range for the Hamiltonian parameters. Notably, the observed degeneracy patterns at the lowest energies hint at an emergent symmetry-breaking state, underscoring the delicate interplay between geometric frustration and longer-range interactions in the hyperkagome lattice. Our work provides insights into the mechanism by which next-nearest-neighbor exchange can stabilize unconventional ground states and opens pathways for refining experimental searches for exotic magnetic phases in rare-earth-based materials.

Flat bands and ferromagnetic fluctuations via orbital-selective electron correlations in Mn-based kagome metal

S. Samanta[1,2], H. Park[3], C. Lee[4], S. Jeon[3], H. Cui[5], Y.-X. Yao[6], J. Hwang[3], K.-Y. Choi[3], and H.-S. Kim[1]*

[1]Dept. of Semiconductor Physics and Institute of Quantum Convergence Technology, Kangwonn National Univ., Chuncheon 24341, Korea
[2]Center for Extreme Quantum Matter and Functionality, Sungkyunkwan Univ., Suwon 16419, Korea
[3]Dep. of Physics, Sungkyunkwan Univ., Suwon 16419, Korea
[4]Dep. of Physics, Chung-Ang Univ., Seoul 06974, Korea
[5]Dep. of Physics and Astronomy and Institute of Applied Physics, Seoul National Univ., Seoul 151-747, Korea
[6]Ames National Lab. U.S. Dep. of Energy, Ames, IA, 50011, USA
Email*: heungsikim@kangwon.ac.kr

Kagome lattice has been actively studied for the possible realization of frustration-induced two-dimensional flat bands and the resulting correlation-induced phases. The search for kagome systems with a nearly dispersionless flat band close to the Fermi level is an ongoing study. By combining theoretical and experimental tools, here we present Sc3Mn3Al7Si5 as a novel realization of correlation-induced almost-flat bands in the kagome lattice near the Fermi level. Our magnetic susceptibility, 27Al nuclear magnetic resonance, transport, and optical conductivity measurements indicate a correlated metallic phase with tantalizing ferromagnetic instability. Our dynamical mean-field calculations suggest that such ferromagnetic instability observed originates from the formation of nearly flat dispersions close to the Fermi level, where electron correlations induce strong orbital-selective renormalization and manifestation of the kagome-frustrated bands. In addition, a significant negative magnetoresistance signal is observed, which can be attributed to the suppression of flat-band-induced ferromagnetic fluctuation, which further supports the formation of flat bands in this compound. These findings broaden a new prospect to harness correlated topological phases via multiorbital correlations in 3d-based kagome systems [1].

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Ab-initio Dynamics of Electrons and Nuclei in Solids

Chung-Yu Wang

Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

Email: chungyuwang0110@gate.sinica.edu.tw

Based on the intuitive picture that the electrons instantaneously adjust to the nuclear motions, the adiabatic approximation is one of the most important cornerstones of modern condensed-matter. However, there exist plenty of intriguing phenomena that cannot be described within the framework of the adiabatic approximation. In solids, novel and fascinating non-adiabatic phenomena can be observed using ultra-short and intense laser pulses. Such laser pulses can give rise to structural phase transitions and light-induced superconductivity. We present two *ab-initio* approaches aiming for a reliable theoretical description of the non-adiabatic process in solids. We first discuss electron dynamics in solids within a given classical nuclear trajectory[1]. Under this semi-classical framework, we extend the concept of the Born effective charge to the dynamical regime and discuss the linear response function of electrons induced by nuclear motion. Lastly, we present our fully quantum mechanical approach dealing with small amplitude nuclear motions in solids. Applying Wick's theorem to the square of the Fröhlich Hamiltonian, we derive a set of two coupled Bogoliubov equations[2]. Solving these coupled Bogoliubov equations, we can obtain the correct band gap renormalization of diamond and silicon and the superconducting gaps of niobium and MgB_2.

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Noncollinear DFT+U+V and Self-Consistent Hubbard Parameters for Fully Relativistic Pseudopotentials

Wooil Yang[1], Young-Woo Son[1]

[1]Korea Institute for Advanced Study, Seoul, Republic of Korea
Email: yspacefirst@kias.re.kr

We present an *ab initio* computational method that extends conventional DFT+*U* approaches by incorporating both on-site and inter-site Hubbard corrections (DFT+*U*+*V*) [1] within a noncollinear framework designed for fully relativistic pseudopotentials [2]. In our method, the Hubbard parameters are determined self-consistently via a Hartree–Fock-based formalism within the self-consistent field procedure [3,4], thereby treating local and non-local Coulomb interactions on an equal footing while mitigating self-interaction errors inherent in standard exchange-correlation functionals. By extending this Hartree–Fock-based formalism to include spin–orbit coupling effects, our scheme accurately predicts physical properties such as spin–orbit splitting, hole effective masses in semiconductor valence bands, and inversion energies in topological insulators, which accuracies comparable to *GW* methods [5]. Benchmark calculations on two-dimensional systems, including Bi_2Se_3 and Bi_2Te_3 up to eight quintuple layers, demonstrate that our approach not only improves predictive reliability but also requires only a moderate increase in computational cost compared to conventional DFT. This work thus offers an efficient and robust framework for studying large-scale correlated materials with pronounced relativistic effects.

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Molecular Doping Strategies for Tailoring the Electronic and Optical Properties of 2D Semiconductors

Jyh-Pin Chou[1]*, Li-Sheng Lin[1], Chih-Piao Chuu[2]

[1]Graduate School of Advanced Technology, National Taiwan University, Taipei 106319, Taiwan

[2]Corporate Research, Taiwan Semiconductor Manufacturing Company, Hsinchu 30091, Taiwan

*Email: jpchou@ntu.edu.tw

The development of two-dimensional (2D) materials, including silicon carbide (2D SiC) and transition metal dichalcogenides (TMDs), such as tungsten diselenide (WSe2) and molybdenum disulfide (MoS_2), has opened new avenues for next-generation electronic and optoelectronic devices. These materials exhibit exceptional electronic and thermal properties, with 2D SiC maintaining the advantageous characteristics of bulk SiC in a honeycomb lattice and TMDs demonstrating layer-dependent electronic structures and strong spin-orbit coupling. While conventional atomic doping methods often induce structural distortions, molecular doping presents a precise approach for modulating charge carrier type and concentration without significantly altering the host material's geometric and electronic structure.

First-principles calculations reveal that molecular doping effectively tunes the electronic and optical properties of 2D SiC, WSe2, and MoS2. Specifically, tetrathiafulvalene (TTF) functions as an n-dopant, while cyano-based acceptors such as F4TCNQ, CN6-CP, and TCNQ serve as p-dopants for these materials. Moreover, an external perpendicular electric field provides an additional degree of control, modulating charge transfer and the relative energy alignment between molecular states and the host band edges. Notably, molecular adsorption enhances optical absorption in the visible range, further expanding the applicability of these hybrid systems.

These findings underscore molecular doping as a powerful strategy for engineering the electronic and optical properties of 2D semiconductors, offering new design principles for high-performance nanoelectronics and optoelectronics.

Exploring Quantum Dynamics via Tensor Network and Complex Time Evolution

Hyun-Yong Lee[1,2] and Heung-Sik Kim[3]

[1] *Division of Semiconductor Physics, Korea University, Sejong 30019, Korea*
[2] *Department of Applied Physics, Graduate School, Korea University, Sejong 30019, Korea*
[3] *Department of Semiconductor Physics, Kangwon National University, Chuncheon 24341, Republic of Korea*

We present a tensor network approach to quantum dynamics based on complex time evolution, which effectively suppresses the rapid entanglement growth commonly encountered in real-time simulations. This method significantly enhances computational efficiency, enabling accurate studies of long-time dynamics. As a benchmark, we apply this approach to the transverse-field Ising model and extract the dynamical critical exponent at the quantum critical point with high precision. Furthermore, we compute the spectral function of the XXZ model with high resolution, demonstrating the capability to resolve low-energy excitations over extended timescales. In both cases, our method outperforms conventional real-time evolution in terms of stability and efficiency[1]. Building on these results, I will also discuss a tensor network-based impurity solver for dynamical mean-field theory (DMFT) that leverages complex-time evolution.

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Low-Dimensional Electronic Structures in Bulks for Improved Thermoelectric Efficiency

Te-Hsien Wang

Institute of Nanoscience, National Chung Hsing University, Taichung City 40227, Taiwan
Department of Physics, National Chung Hsing University, Taichung City 40227, Taiwan
Email: thwang@phys.nchu.edu.tw

Thermoelectric (TE) materials, capable of directly converting heat into electricity, have emerged as key candidates for energy harvesting and waste heat recovery applications. In this talk, I will discuss how low-dimensional electronic features can be leveraged to enhance TE performance in bulk materials, focusing on PbTiO3 and GeTe-based compounds. Through first-principles calculations complemented by experimental insights, we find that these bulk materials exhibit electronic behavior akin to low-dimensional systems. Such behavior results in increased band degeneracy and improved TE properties. The highly anisotropic band structures—featuring flat dispersion in specific crystallographic directions and strong dispersion in others—generate a density of states that mimics that of nanostructures while avoiding the drawbacks of subband splitting. These findings open new possibilities for designing bulk materials with low-dimensional-like electronic structures, enabling significant advancements in TE performance and energy conversion efficiency.

Simulating Electronic Structure of Defect without Supercell Calculations

Tae In Kim and Seunghoon Lee*

Department of Chemistry, Seoul National University, Seoul 08826, South Korea
Email*: seunghoonlee@snu.ac.kr

Understanding the electronic structure of defects in material systems is important for advancing quantum materials, as defect sites can function as qubits or key quantum elements. The coherence time of defect-based qubits, along with other essential properties, is governed by their electronic structure and couplings with phonons. Thus, efficient and accurate ab-initio electronic structure methods for the defects can accelerate the development of materials tailored for quantum computing, spintronics, and next-generation quantum technologies.

The electronic structure of defects is commonly studied using supercell calculations. The supercell calculations provide a detailed analysis of defect-induced electronic states, charge redistribution, and modifications in the band structure. However, the periodic replication of the defect can lead to unintended interactions between neighboring images due to periodic boundary conditions, resulting in inaccuracies in defect level calculations. One common way to mitigate these artificial interactions is by increasing the supercell size. In addition, employing hybrid functionals such as HSE06 can further suppress these effects. However, both approaches significantly increase computational cost. Alternatively, correction schemes like the Makov-Payne correction are often used for charged defects to improve accuracy. In this talk, we introduce a novel simulation method that fundamentally overcomes the limitations of supercell calculations. By leveraging iterative unit-cell-level computations, our approach enables accurate and efficient simulations of defect electronic structures.

Machine Learning Approaches for Material Microstructures: from classical to quantum machine learning

Chun-Wei Pao

Research Center for Applied Sciences, Academia Sinica, Taipei 115201, Taiwan
Email: cwpao@gate.sinica.edu.tw

In recent years, machine learning (ML) has attracted significant attention for its ability to efficiently identify correlations between complex inputs and outputs. In this talk, I will present our efforts to leverage ML for exploring the microstructures of complex materials, including mixed-ion perovskites, 2D perovskites, and high-entropy intermetallic alloys. We demonstrate that ML-enabled energy models can predict the energetics of these materials with high fidelity compared to DFT calculations, providing a highly efficient surrogate for systematically exploring configurational spaces and extracting microstructural properties such as phase stabilities and dislocation dynamics. Finally, I will discuss our latest work on extending these ML energy models to quantum circuits, achieving reasonable predictive power with significantly fewer trainable parameters.

Gate-controllable array of quantum dots in twisted trilayer *h*-BN

Kunihiro Yananose[1], Changwon Park[1,2] and Young-Woo Son[1]*

[1] Korea Institute for Advanced Study, Seoul, 02455, Republic of Korea
[2] Department of Physics, Ewha Womans University, Seoul, 03760, Republic of Korea
Email*: hand@kias.re.kr

Trilayer hexagonal boron nitride (h-BN) has two opposite polar stackings (so-called, ABC and ACB) and two distinct non-polar ones (ABA and ACA). In this talk, we show that for the marginally twisted trilayer h-BN of which the twist angle is tiny, a slight energetic difference between the polar and non-polar stackings leads to the variety in the stacking patterns, such as spontaneously symmetry broken kagome-type pattern [1]. Similar lattice reconstructions were demonstrated in twisted graphene trilayers [2]. Our simulation demonstrates these patterns and their ferroelectric controllability where the polar stacking area can expand or shrink by applied electric field, including the transition between different patterns [1]. In addition, large-scale tight-binding calculations show that the vertex sites of the patterns can host the localized quantum dot states. We demonstrate that for some stacking orders, the regular array of quantum-dot states at different vertices can be controlled by external electrical means, thereby providing exciting possibilities for quantum device applications.

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Numerical approach to superconductivity and stripes in the Hubbard model

Chia-Min Chung

Department of Physics, National Sun Yat-sen University, Kaohsiung, Taiwan
Center for Theoretical and Computational Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan
Physics Division, National Center for Theoretical Sciences, Taipei 10617, Taiwan
Email: chiaminchung@gmail.com

The Hubbard model is an iconic model in quantum many-body physics and has been intensely studied, especially since the discovery of high-temperature cuprate superconductors. The development of advanced numerical techniques, such as tensor networks and quantum Monte Carlo, now enables highly accurate simulations of correlated electron systems. In this talk, I will introduce our works in numerical studies on the two-dimensional Hubbard model. Recently, we found superconductivity in both the electron- and hole-doped regimes of the two-dimensional Hubbard model with next-nearest neighbor hopping. In the electron-doped regime, superconductivity was weaker and was accompanied by antiferromagnetic Néel correlations at low doping. The strong superconductivity on the hole-doped side coexisted with stripe order, which persisted into the overdoped region with weaker hole-density modulation. These stripe orders varied in fillings between 0.6 and 0.8. Our results suggest the applicability of the Hubbard model with next-nearest hopping for describing cuprate high–transition temperature (Tc) superconductivity.

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From Jahn-Teller Distortions to Spin-Orbital Entanglement: Pathways to Mott Metal-Insulator Transition

Choong H Kim

Korea Institute for Advanced Study, Seoul, Republic of Korea
Email: CHOONGHKIM@kias.re.kr

The Mott metal-insulator transition (Mott MIT) is one of the most prominent emergent phenomena in strongly correlated systems. Unlike conventional band insulators, Mott MIT arises from the interplay of Coulomb interaction, spin-orbit coupling, and lattice distortion, leading to novel phase transitions and electronic states. In multi-orbital systems, the lifting of orbital degeneracy plays a crucial role in determining the MIT. This can be driven by Jahn-Teller distortion, spin-orbit coupling, or a complex interplay of Hund's coupling and Coulomb U, which can either compete or cooperate in shaping the phase transition. In this presentation, we will discuss how key factors such as Coulomb U, lattice distortion, Hund's coupling, and spin-orbit coupling interact to produce intriguing phase diagrams in strongly correlated materials. Specifically, we will focus on two systems: the $CuAl_2O_4$ spinel, where strong spin-orbit coupling leads to a novel spin-orbital-entangled state, and monolayer $SrRuO_3$, where a new type of Jahn-Teller distortion drives the metal-insulator transition. These cases highlight the rich physics underlying Mott MIT and provide insights into the broader implications for correlated electron systems.

Structure-imposed Electronic and Topological Properties in One- and Two-Dimensional Conjugated Carbon Systems

Tsai-Jung Liu

Institute of Chemistry, Academia Sinica, Taiwan
Email: trishaliu83@gmail.com

The honeycomb lattice of graphene is renowned for its intriguing topologically non-trivial properties, including the presence of massless Dirac fermions. These properties are closely linked to the material's geometric structure, such as lattice symmetries and edge configurations. To explore materials beyond graphene, researchers can utilize bottom-up synthesis techniques to create different two-dimensional (2D) polymers or various nanoribbons with well-defined edge conformations. This approach avoids the challenges associated with synthesizing highly strained three- or four-membered rings that typically arise when creating carbon allotropes.

Among theoretical methods, the tight-binding (TB) approach is a straightforward and effective tool for studying the electronic and topological properties of π-conjugated systems. In this presentation, I will demonstrate how the TB method can be used to connect structural features to electronic properties. This serves as a crucial first step in material design before progressing to more complex structures or higher-level calculations, such as density functional theory (DFT).