**Computational Modeling of Nanoelectronics and Emerging Materials**

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 Using first-principles calculations based on density functional theory, we investigate electronic transport through carbon-, silicon- and transition metal dichalcogenide (TMD)-based nanojunctions for nanoelectronic applications. Effects of doping, contacting and quantum interfering are addressed. We also study the efficiencies of CO2 photoconversion and hydrogen evolution reaction in TMD and oxides for sustainable-energy applications. Effects of nanoparticle-adsorbing and material-configuring are highlighted. Moreover, we explore the plasmonic properties of complex transition metal nitrides for photonic applications.