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SEMINAR SERIES

Tuesday, November 1st, 2022
Seminar Presentation: 11:00am – 12:00pm PDT
SME room 248

"First-Principles Many-Body Theory and Quantum Dynamics for Materials in Quantum Information Science"

Dr. Yuan Ping, PhD

Associate Professor in Department of Chemistry and Biochemistry
and Affiliated Professor in Physics Department
University of California, Santa Cruz

Abstract: Stable, scalable, and reliable quantum information science (QIS) is poised to revolutionize human well-being through quantum computation, communication and sensing. In this talk, I will show our recent development on first-principles computational platforms to study quantum coherence and optical readout as critical processes in QIS in solid-state materials, by combining first-principles many-body theory and open quantum dynamics.

First, we will show how we reliably predict energetics, electronic and optical properties of spin defects and their host two-dimensional materials from first-principles many-body theory, which accurately describes highly anisotropic dielectric screening and strong many-body interactions. In particular, we will show how we predict spin-dependent optical contrast for information readout of spin qubits by computing exciton radiative and phonon-assisted nonradiative as well as spin-orbit induced intersystem crossing kinetic rates from first-principles.

Next, we will introduce our recently developed real-time density-matrix dynamics approach with first-principles electron-electron, electron-phonon, electron-impurity scatterings and self-consistent spin-orbit coupling, which can accurately predict spin and carrier lifetime and pump-probe Kerr-rotation signatures for general solids. As an example, we will show our theoretical prediction on Dirac materials under electric field with extremely long spin lifetime and spin diffusion length, and distinct spin and carrier relaxation behavior in halide perovskites. This theoretical and computational development is critical for designing new materials promising in quantum-information science and spintronics applications.

Biosketch: Yuan Ping received her B.Sc. degree from University of Science and Technology of China in 2007, Ph.D. from UC Davis in 2013, and materials postdoctoral fellow at Caltech in 2016. From then she is an assistant professor in chemistry and affiliated professor in physics at UC Santa Cruz, and promoted to be an associate professor with tenure in 2022. Her research group focuses on developing and employing first-principles many-body theory and quantum dynamics for materials applications. Ping is a recipient of Alfred Sloan Research Fellow (2022), DOE Computational Chemistry Science Award (2022), NSF CAREER Award (2022), Air Force YIP award (2021), and ACS COMP OpenEye Award (2021). Her group website: https://yuanping.chemistry.ucsc.edu/