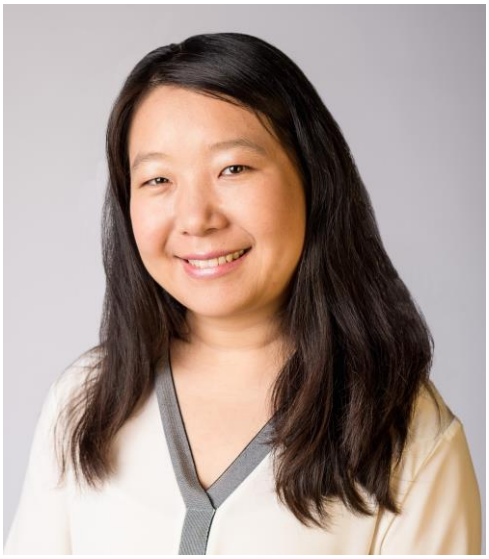
UCLA College | Physical Sciences Chemistry & Biochemistry

THEORETICAL PHYSICAL CHEMISTRY SEMINAR



Professor Yuan Ping

Department of Chemistry & Biochemistry
University of California, Santa Cruz

Monday, Feb. 08, 2021
4:00 PM PST
Zoom

First-Principles Materials Prediction: From Sustainability to the Quantum Information Age

Theory-guided materials design is vital to the advancement of sustainability and quantum information science. First-principles theory entirely based on quantum mechanics without prior input parameters is the perfect tool. In order to reliably predict exotic quantum materials and out-of-equilibrium processes, many-body physics and quantum kinetic theory are important to bridge with first-principles methods.

In this talk, I will discuss our development on theory and numerical codes on many-body perturbation theory (MBPT), for accurate prediction of optical excitation and exciton recombination[1,2,3]. We will discuss how we use these methods to solve material problems in photoelectrochemical applications and predict spin qubit properties for quantum information science[4,5]. In particular, we will show an example on how substrate screening affects interfacial charge transfer and exciton energies, with our recently developed technique based on MBPT that applies for arbitrarily lattice-mismatched interfaces without strain[6].

Next, I will show our recent method development on real-time open quantum dynamics with coupled spins, electrons, photons and phonons based on first-principles density-matrix approach[7,8]. We will discuss its important applications on understanding valley dynamics, spin transport as well as ultrafast coupled spin and carrier dynamics at finite temperature. This method will offer new and unbiased insights for spin and valley relaxation and decoherence in general systems, and determine design rules for new materials with ideal physical properties for spintronics, valleytronics, and quantum information science.

Please contact nikke@chem.ucla.edu for additional information.