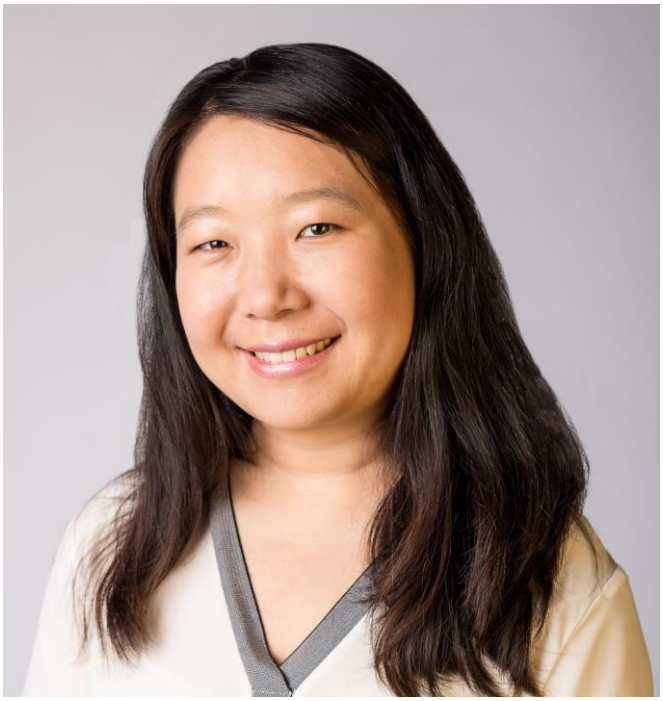
UCLA College | Physical Sciences Chemistry & Biochemistry

Theoretical Physical Chemistry Seminar



Professor Yuan Ping

Dept. of Chemistry & Biochemistry

UC Santa Cruz

Thursday, Dec. 3, 2020

12:00 PM

Zoom

"First Principles Many-Body Theory and Quantum Dynamics for Materials Prediction"

Materials prediction is the ultimate solution for ending blind experimental search within an expansive material parameter space. First-principles theory entirely based on quantum mechanics without prior input parameters is the perfect tool for new material design. In order to predict exotic quantum materials and out-of-equilibrium processes, many-body physics and quantum kinetic theory are needed to bridge with first-principles methods.

In this talk, I will discuss the past development on theory and numerical codes of solving the Bethe-Salpeter equation without explicit empty states, for accurate prediction of optical excitation and exciton recombination. I will show the recent developments on radiative and phonon-assisted nonradiative exciton recombination in two-dimensional materials and spin defects. Next, I will show our recent method development on real-time quantum dynamics with coupled spins, electrons, photons and phonons based on first-principles density-matrix approach. This method will offer new and unbiased insights for spin relaxation and decoherence in general systems, and determine design rules for new quantum materials with ideal physical properties for spintronics and quantum information science.

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