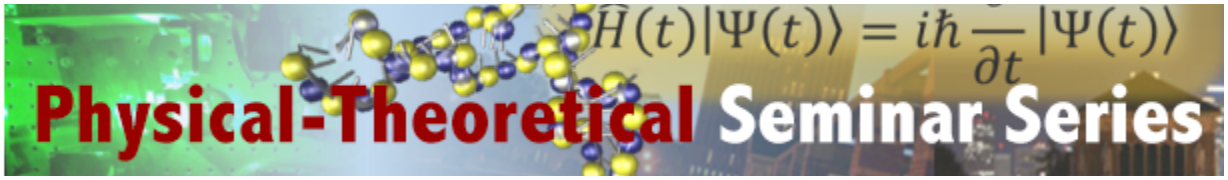

Monday, January 25, 2021 at 12:00 pm
Zoom Link for Seminar & Student Meeting:
https://usc.zoom.us/j/94503521900

Professor Yuan Ping

Department of Chemistry & Biochemistry
University of California Santa Cruz

First-Principles Materials Prediction: from Sustainability to Quantum Information Science

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 our past development on theory and numerical codes of solving Bethe-Salpeter equation for accurate prediction of optical excitation and radiative and nonradiative exciton recombination[1,2,3]. We will show examples using these methods to study materials in photoelectrochemical application and spin defects in two-dimensional systems in quantum information science[4].

Next I will show our recent method development on real-time quantum dynamics with coupled spins, electrons, photons and phonons based on a first-principles density-matrix approach[5,6]. 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.

[1] F. Wu, D. Rocca and Y. Ping, *Journal of Materials Chemistry C*, **7**, 12891, (2019)
[2] F. Wu, T. Smart, J. Xu, Y. Ping, *Physical Review B*, **100**, 081407(R) (2019)
[3] Y. Ping, D. Rocca, G. Galli, *Chem. Soc. Rev.* **42**, 2437 (2013)
[4] F. Wu, A. Galatas, R. Sundararaman, D. Rocca, and Y. Ping**,** *Physical Review Materials,* **1**, 071001(R), (2017).
[5] J. Xu, A. Habib, S. Kumar, F. Wu, R. Sundararaman, and Y. Ping, *Nature Communications*, **11**, 2780, (2020)
[6] J. Xu, A. Habib, R. Sundararaman, and Y. Ping, *Phys. Rev. X*, under review, arXiv: 2012.08711 [cond-mat-mtrl-sci], (2021)

Hosted by Professor Oleg Prezhdo
The scientific community is invited

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