UCMERCED UNIVERSITY OF CALIFORNIA School of Natural Sciences

CHEMISTRY SEMINAR 291

First-principles Study of Complex Defects: From Polaronic Conduction to Single Photon Emission

Yuan Ping
Department of Chemistry and Biochemistry
University of California, Santa Cruz

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For more information contact:
David Strubbe
dstrubbe@ucmerced.edu

ABSTRACT

In this talk, I will discuss effects of defects on two different problems from first-principles calculations: one is to boost small polaron conduction in transition metal oxides by atomic doping, using Mo doped $BiVO_4$ and Li doped CuO as examples;
another is charge defects in two dimensional (2D) materials as single photon emitters for quantum information applications.

We will discuss our recent methodology development in coupling Landau-Zener theory with random walk sampling for small polaron mobility in doped metal oxides, and excited state dynamics of charged defects in ultrathin 2D systems from many body perturbation theory. Then we will show you how we use our methodology to discover good dopants/defects for energy conversion and quantum information applications.

BIO:

Yuan Ping received her B.Sc. degree in Chemical Physics from University of Science and Technology of China, China, in 2007 and her Ph.D. in physical chemistry from University of California, Davis in 2013. She was a materials postdoctoral fellow in the DOE energy hub- Joint Center for Artificial Photosynthesis at California Institute of Technology from 2013 to 2016. In 2016, she joined the faculty at UC Santa Cruz as an assistant professor. Ping's recent research interests focus on first-principles methodology development on excited-state dynamics for solids, in particular, from many-body perturbation theory with improved numerical efficiency and accuracy, and charged defect properties as color centers in low-dimensional systems and dopants' effect on carrier transport in polaronic oxides. Ping has authored over 20 peer-reviewed publications, and she is a recipient of a Hellman Fellowship 2018.