

UNIVERSITY OF CALIFORNIA, IRVINE

THE DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

Is Proud to Host a Seminar by:

PROFESSOR BRYAN M. WONG

Materials Science and Engineering Program
Depts. Of CEE, Physics & Astronomy, and
Chemistry
University of California, Riverside

Thursday, February 9, 2023

2:00-3:20 PM

Location:

McDonnell Douglas Engineering Auditorium

PROBING ELECTRON DYNAMICS OF COMPLEX MATERIAL SYSTEMS IN REAL TIME

Abstract: Light-harvesting systems and electronic materials continue to garner significant attention due to their importance in energy conversion and modern technological advances. However, several challenges exist in improving their performance: these multifunctional electronic systems are complex, coupled, many-body systems with structural and electronic interactions with their surrounding environments. To address these issues, we have developed several computational approaches based on real-time, time-dependent density functional theory (RT-TDDFT) to directly predict and probe these complex material systems. Our approach significantly differs from conventional DFT methods in that we can directly calculate real-time dynamical effects in the presence of strong interactions with the surrounding environment. Furthermore, recent RT-TDDFT developments in my group allow us to calculate the electronic and structural properties of large systems (~10,000 atoms), whereas conventional DFT approaches are typically limited to only hundreds of atoms. Using these RT-TDDFT capabilities (in conjunction with custom computational hardware developed in my group), I will highlight our recent work on representative light-harvesting systems and complex materials. By treating these large systems at a quantum-mechanical level of detail, we show that the energy-transfer dynamics in these materials are surprisingly rich and complex. Most importantly, these time-resolved studies provide a new approach to probe real-time energy-transfer mechanisms to understand and tailor these complex systems for realistic engineering applications.

Bio: Prof. Bryan M. Wong received BS (2001) degrees in physics and chemistry from Rice University and received a PhD (2007) in chemical physics from the Massachusetts Institute of Technology (M.I.T.). Prof. Wong is a full Professor in the Materials Science & Engineering Program, Department of Physics & Astronomy, and Department of Chemistry at the University of California-Riverside. Prof. Wong has published over 190 scientific journal articles and is the recipient of a Department of Energy (DOE) Early Career Award, an R&D 100 Award, the ACS COMP Outstanding Junior Faculty Award, and a 2022 HPCWire Award for TDDFT calculations. Prof. Wong is the lead PI on a new DOE SciDAC center at UC Riverside on large-scale TDDFT calculations for material systems.