



PHYSICS COLLOQUIUM:

Quantum Molecular Dynamics of Metal-Insulator Transition In Correlated Electron Systems

Gia-Wei Chern

Associate Professor, Physics
University of Virginia

Date:

9/10/2021

Time:

10:30 AM-11:50 AM

Link:

Please email
snsgradstaff@ucmerced.edu
for Zoom link and
passcode.

About The Speaker:

Education and Training

National Taiwan University Electrical Engineering B.S. 1996

National Taiwan University Optoelectronics Engineering Ph.D. 2001

Johns Hopkins University Physics Ph.D. 2009

Research and Professional Experience

2015 – Present Assistant Professor of Physics, University of Virginia

2012 – 2015 J. R. Oppenheimer Fellow, Los Alamos National Laboratory

2010 – 2012 ICAM Postdoctoral Fellow, U. Wisconsin-Madison/Los Alamos

2008 – 2010 Postdoctoral Research Associate, University of Wisconsin at
Madison

Abstract:

In this talk, I will present our recent efforts on dynamical simulations of correlated electron systems. I will first discuss new quantum molecular dynamics (QMD) methods based on advanced many-body techniques, such as Gutzwiller/slave-boson and dynamical mean-field theory, that are capable of modeling strong electron correlation phenomena. We apply our new QMD to simulate the correlation-induced Mott transition in a metallic liquid, and the nucleation-and-growth of Mott droplets in Hubbard-type models. I will also discuss the implementation of the ab initio Gutzwiller MD for simulating hydrogen liquids under high pressure. To overcome the obstacle of huge computational complexity in such large-scale simulations, I will discuss how simulation efficiency can be significantly improved with the aid of modern machine learning methods. In particular, deep-learning neural-network holds the potential of achieving large-scale quantum-accuracy simulation of correlated systems without the electrons.