

JOINT SPECIAL COLLOQUIUM  
BY COLLEGE OF SCIENCE AND COLLEGE OF ENGINEERING

# Modeling Quantum Information and Quantum Materials Problems

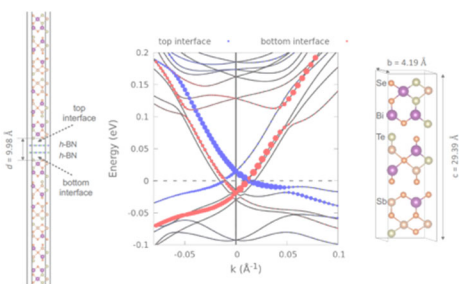
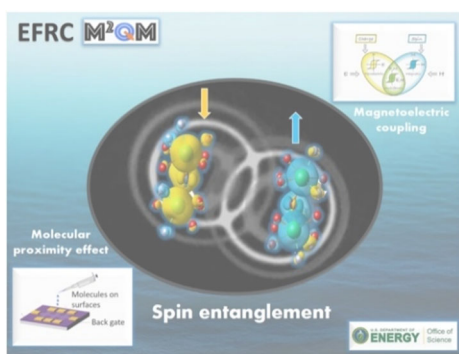
Prof. Hai-Ping Cheng, University of Florida

**Thursday, May 19, 2022; 3:00 to 4:00 p.m.**

**Hosts: Arun Bansil and Swastik Kar**

**Zoom meeting link:**

<https://northeastern.zoom.us/j/91068308741>



I will discuss how large-scale computational efforts based on model Hamiltonians informed by first-principles simulations with inputs from experiments have allowed us to gain unprecedented clarity in the microscopic mechanisms underlying macroscopic properties of materials. Such an approach is critically important for exploration of viable qubit candidates beyond the current technologies which are based on superconductors and ion traps. Covering six orders of magnitude in energy scales, magnetic couplings present a fundamental challenge to first-principles calculations. In this talk, I will highlight some of our recent work concerning inter- and intra-molecular spin-spin couplings, magneto-electric couplings, magnetic molecules on substrates and in junctions, and decoherence. I will also show results from simulations of interfaces and vertical junctions that consist of two topological insulators and 2D materials.



Dr. Hai-Ping Cheng is a Professor of Physics and Director of the Quantum Theory Project at the University of Florida. She currently leads the DOE Energy Frontier Research Center (EFRC) for Molecular Magnetic Quantum Materials (M<sup>2</sup>QM). She received her Ph.D. from Northwestern University (1988), was a postdoctoral researcher at the University of Chicago (1989-1991), and a research scientist at the Georgia Institute of Technology (1992-1994). Her research interests include magnetic molecules for quantum information sciences, interface phenomena and transport across tunneling junctions, and reduction of thermal noise in amorphous oxides.