

Friday, February 18, 2022

4:10 – 5:00 PM

Barnard Hall 103



Entangled and Unentangled Quantum States: New Methods and Applications

Martín A. Mosquera

Department of Chemistry and Biochemistry, MSU

Abstract:

Determining the quantum properties of electronic states of materials and molecules is a common driving force for the application, improvement, or creation of computational methods. In this talk we discuss the following: 1) challenges in the field of single-electron theory (e.g., density functional theory) to address quantum entanglement and the description of weakly interacting molecular systems. We show a simple modification to the common theory that provides an intriguing way to approach the mentioned challenges. 2) Computing interactions between entangled photon pairs and molecules/0D systems: This is an exciting subarea of optical quantum science where electronic quantum states of 0D systems are studied. Finally, 3), Raman calculations of 2D materials: We present results where theory and experiment, a powerful alliance at MSU, work together to interpret tip-enhanced Raman measurements of alloyed single-layer transition metal dichalcogenides. The use of high-performance computing led to theoretical Raman spectra that are consistent with state-of-the-art experiments.

Host: Anton Vorontsov

** Refreshments served in the Barnard second floor atrium at 3:45 **