

PHYSICAL CHEMISTRY SEMINAR

Martin A. Mosquera

Associate Professor | Department of Chemistry and Biochemistry |
Montana State University - Bozeman

Electronic Structure of Iron-Sulfur Clusters and 2D Materials

Iron-sulfur clusters conduct a wide variety of biochemical reactions that are conserved across all domains of life. The quantum spin structure of their reactive ligands can be probed by magnetic hyperfine spectroscopy, which reveals catalytic intermediates in these processes. The theoretical prediction of hyperfine couplings, however, requires either advanced methods for strongly correlated systems or Hamiltonian modeling based on symmetry-broken electronic structure calculations. In the first part of the talk, we show that adding electron-transfer interactions to the Heisenberg-Dirac-Van Vleck Hamiltonian leads to a quantitative explanation of hyperfine coupling constants at active organic ligand sites, in agreement with available experimental results, which opens the way to describing cutting-edge systems. For the second part of the talk, we consider

Two-Dimensional Materials, which are also promising for a wide variety of optoelectronic applications in quantum and semiconductor technologies. My group has worked in recent years on using machine learning, band structure theory, and parameter-free quantum modeling to investigate multiferroic phenomena, twistrionics, and exciton functionalities. We discuss progress in these directions where we show that machine-learned potentials are effective in describing phonon transport and structural defects, and where band theory is reliable for supporting and explaining the experimental modulation of excitons in twisted transition-metal dichalcogenide bilayers.

PHYSICAL CHEMISTRY SEMINAR

Martin Mosquera's Biography

Martin A. Mosquera is an Associate Professor in the Department of Chemistry and Biochemistry at Montana State University, Bozeman. He received his B.S. in Chemical Engineering from Universidad del Valle in Cali, Colombia, and his Ph.D. in Chemistry from Purdue University in 2014, where he worked on density functional theory with Prof. Adam Wasserman. From 2015 to 2020 he was a postdoctoral fellow at Northwestern University with Profs. George Schatz and Mark Ratner, working on theory and algorithms for the optical and catalytic properties of molecules, clusters, and materials. He joined Montana State University in 2020.

His group works on electronic structure theory, including time-dependent methods, and applies it to a range of problems such as the spin structure and catalytic intermediates of iron-sulfur clusters, Bose-Hubbard systems relevant to quantum information science, and the optical, thermal, and ferroelectric properties of two-dimensional materials. Much of this work is carried out in close collaboration with experimental colleagues, and it owes a great deal to the students and postdocs who have been part of the group. The group's research has been supported by a US Department of Energy Early Career Award (2024) and a Camille Dreyfus Teacher-Scholar Award (2025). At Montana State he teaches physical chemistry, quantum mechanics, and computational chemistry.