SPECTROSCOPIC AND ELECTRONIC STRUCTURE STUDIES OF MOLECULAR ELECTRON TRANSPORT

INTRODUCTION TO OUR RESEARCH

WHAT IS MOLECULAR ELECTRONICS? Molecular electronics focuses on the use of molecules as building blocks and functional units in the construction of tailored nanoscale electronic components. The research uses a combination of molecular synthesis, spectroscopy, current measurement, device construction, and theory/computations and bridges the traditional research areas of materials science, physics, and chemistry. Researchers in molecular electronics are developing connections between magnetic exchange, electron transfer/transport, molecular conductance, and electronic coupling in molecular systems to provide a basis for understanding electronic structure contributions to the development of molecular electronic components. When molecules bridge metallic electrodes, the molecular contact geometry is often unknown. Thus, researchers typically construct conductance histograms comprised of many thousands of individual measurements in order interpret single molecule conductance properties. In these experiments, it is difficult to assess which molecular geometry(ies) are productive for transport relative to the electrodes. Molecules can be designed for use in device configurations to function as diodes or current rectifiers, and their efficiency is determined by the rectification ratio. For molecular rectifiers under bias conditions, the preferred current direction with respect to the molecular dipole and the applied bias is often unknown. How molecular bridge geometries affect conductance represents critical a gap in the knowledge base that we aim to address in our research program.

WHAT ARE WE DOING? Indeed, there is tremendous potential for molecular science to advance new device technologies, and we are addressing specific questions related to molecular conductance and rectification. These studies will benefit society and chemistry-related disciplines by expanding the knowledge base and contributing to a broader understanding of molecular electron transport that will drive next generation molecular and molecule-based technologies. Our long-term goal is to understand how molecular design principles can be used to increase our understanding of device-oriented molecular electron transport behavior. A primary goal of the project is to relate computed molecular conductance values with experimental spectroscopic and magnetic data to gain new insight into electronic structure contributions to single-molecule conductance and molecular rectification. We use a combination of magnetic susceptibility measurements, magnetic resonance techniques, excited state spectroscopies, ligand K-edge X-ray absorption spectroscopy, electronic structure computations, electron transport calculations, and molecular synthesis to determine bridge-dependent magnetic exchange coupling constants ($J_{D\text{-}B\text{-}A}$) in donor-bridge-acceptor biradicals and how they relate molecular conductance, quantum interference, and molecular rectification. Our understanding of electronic structure contributions to these exchange interactions will dramatically a more detailed understanding of molecular electron transport, and pave the way forward for using bespoke molecules in future electronic devices.