MAR15-2014-003823

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Electron Transport, Energy Transfer, and Optical Response in Single Molecule Junctions

ALEXANDER WHITE, Theoretical Division, Los Alamos National Laboratory; Department of Chemistry and Biochemistry, University of California San Diego

The field of molecular electronics has grown significantly since the first measurements of single molecule conductance. The single molecule junction, a device in which two conducting leads are spanned by a single molecule, has become a powerful tool for studying charge transfer at the molecular level. While early experiments were focused on elastic electron conductance, today measurements of vibronic effects, molecular optical response, spintronics, thermal conductance, and quantum interference and decoherence effects are prominent areas of research. These new experimental advancements demand improved theoretical treatments which properly account for the interactions between different degrees of freedom: charge, electronic, vibrational, spin, etc.; all in physically relevant parameter ranges. This talk focuses on using a many-body states based approach to investigate the regime of strong interaction between these degrees of freedom, with relatively weak coupling between the molecule and the electric reservoirs created by the conducting leads. We focused on three related processes, electron transfer, electronic energy transfer and molecular excitation.

In collaboraton with Boris Fainberg, Faculty of Sciences, Holon Institute of Technology; Sergei Tretiak, Theoretical Division, Center for Integrated Nanotechnologies, Los Alamos National Laboratory; and Michael Galperin, Department of Chemistry and Biochemistry, University of California San Diego.