Molecular Junctions

Nanostructure-based solar- and fuel cells, both organic and inorganic, hold promise for efficiently and cheaply converting solar energy into forms convenient for storage and transportation. A primary reason for the currently low efficiency of these devices is the absence of a quantitative picture of the fundamental nonequilibrium electronic structure underlying key processes in solar energy conversion - photon absorption and charge separation, transport, and collection at organic/metal and organic/inorganic interfaces. Single molecule junctions are model interfaces between a single organic molecule connected to macroscopic metallic electrodes, and as such provide an ideal platform for developing the fundamental understanding needed.

In our group, we explore the interplay between local chemistry and many-body effects and how this impacts macroscopic transport and spectroscopic properties of these systems. Potential applications include the design of more efficient molecular rectifiers and single-nanostructure photovoltaics.

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**Thermopower and conductivity in single molecules**

Alison Hatt posted on Mar 28, 2012

In collaboration with Latha Venkataraman at Columbia University, we study junctions of individual amine- and pyradine-based molecules trapped between gold contacts. The Venkataraman group developed a novel setup based on a scanning-tunneling microscope to vary temperature and electrical biases while the molecules remain trapped, allowing them to simultaneously measure conductivity and thermopower.

Comparison of the experimental results to our charge transport calculations reveals an unexpectedly complex relationship between conductance and thermopower arising from chemical details of the metal-molecule contact, not the simple relation usually assumed. These findings critically advance knowledge of molecular-level charge transport, laying the groundwork for molecular-scale engineering of thermoelectric and other energy conversion materials.

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**Related Publications**

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