Energy Transport and Conversion in Organic-Inorganic Heterojunctions Materials

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Hybrid materials made from organic-inorganic constituents has the potential to revolutionize the energy landscapes of organic electronics, thermoelectrics, and photovoltaics. Energy transport and conversion in these devices are heavily influenced by interactions at interfaces. The interface between organic and inorganic moieties is of particular interests as each moiety interacts constructively on the nanoscale to produce enhancements that could not be realized alone. To better understand these interfaces, a simplified heterojunction systems consisting of short (< 3 nm) single-molecules covalently bonded to metal electrodes can be formed using a variety of instruments including a modified scanning tunneling microscope break junction (STM-BJ), conducting atomic force microscope (CAFM), and mechanically (piezoelectric) controlled break junction (MC-BJ). The electronic conductance, thermal conductance, thermopower, and IV characteristics of these heterojunction is currently being investigated (using the above instruments) to understand how to implement interface enhancements for scalable devices. Recently, we have shown that the thermoelectric effect[1] can be realized in single-molecules and, in fact, such a phenomenon better aids in understanding intra-molecular transport[2,3] better than conventional electronic conductance measurements. In addition, we have recently reported that thermoelectric enhancement can be achieved by effectively doping a (noble) metal junction using fullerenes (i.e., C_{60}, PCBM, and C_{70})[4]. More recently, however, we found that molecular junctions with diode characteristics can be realized using monomers of conventional organic polymer solar cells. In response, a systematic study of the molecular components (i.e., end group - electron acceptor – bridge - electron donor - end group) is being conducted in order to identify and control molecular diode behaviors for applications towards more efficient organic solar cells. The forthcoming presentation is aimed at highlighting the fundamentals of energy transport and conversion in organic-inorganic heterojunctions with emphasis on our work in thermoelectric enhancements and electrical rectifying behavior of molecules using our home built STM-BJ, CAFM, and MC-BJ.

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2. K. Baheti *et al.*, *Nano Letters* **8**, 715 (Feb, 2008).
3. J. A. Malen *et al.*, *Nano Letters* **9**, 1164 (2009).
4. J. A. Malen, S. K. Yee, R. A. Segalman, A. Majumdar, *Submitted*