MRSEC SEMINAR SERIES

"Understanding Non-Equilibrium Charge Transport and Rectification at Nanoscale Interfaces."

Understanding and controlling non-equilibrium charge transport across nanoscale interfaces and in supramolecular assemblies is central to developing an intuitive picture of fundamental processes in nanoelectronics, photovoltaics, and other energy conversion applications. In this talk, I will discuss our theoretical studies of finite-bias transport at prototypical organic/metal interfaces, single-molecule junctions, small organic molecules trapped between gold electrodes. I will show how many-body effects influence energy level alignment in these systems, and that simple models of non-local correlations and bias-induced Stark effect on the top of density functional theory lead to quantitative agreement with experiments [1-7]. Finally, I will discuss the implications of this theory in the context of transport in molecular diodes [8]; in particular, how to systematically optimize rectification by tuning the competing energy scales in single-molecule junctions via molecular conformation and asymmetric coupling to electrodes [9,10].

References:
[1] J.B. Neaton et al. Phys. Rev. Lett. 97, 216405 (2006); [2] I. Tamblyn,, et al. Phys. Rev. B, 84, 201402(R) (2011); [3] J. Widawsky, et al. NanoLett. 12, 354 (2012); [4] P. Darancet, et al. NanoLett 12, 6250 (2012); [5] T. Kim, et al. NanoLett. 2, 794 (2014); [6] B. Capozzi, et al. NanoLett 3, 1400 (2014); M. Kotiuga, et al. Nano Letters 15, 449 (2015) [8] A. Aviram and M. A. Ratner, Chem. Phys. Lett. 29, 277 (1974); [9] A. Batra, et al. NanoLett. 13, 6233 (2013); [10] J.A. Smerdon, et al. in preparation.

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