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Abstract for an Invited Paper
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Understanding Non-Equilibrium Charge Transport and Rectification at Chromophore/Metal Interfaces[1]

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Understanding non-equilibrium charge and energy transport across nanoscale interfaces is central to developing an intuitive picture of fundamental processes in solar energy conversion applications. In this talk, I will discuss our theoretical studies of finite-bias transport at organic/metal interfaces. First, I will show how the finite-bias electronic structure of such systems can be quantitatively described using density functional theory in conjunction with simple models of non-local correlations and bias-induced Stark effects. [1-6]. Using these methods, I will discuss the conditions of emergence of highly non-linear current-voltage characteristics in bilayers made of prototypical organic materials, and their implications in the context of hole- and electron-blocking layers in organic photovoltaic [7,8]. In particular, I will show how the use of strongly-hybridized, fullerene-coated metallic surfaces as electrodes is a viable route to maximizing the diodic behavior and electrical functionality of molecular components. 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. Nano Letters 12, 354 (2012); [4] P. Darancet, et al. Nano Letters 12, 6250 (2012); [5] T. Kim, et al. Nano Letters 2, 794 (2014); [6] B. Capozzi, et al. Nano Letters 3, 1400 (2014); [7] J.A. Smerdon, et al. Nano Letters 16, 2603 (2016) [8] J.A. Smerdon, et al. *submitted* (2016).

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