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Theory of Giant Rectification in Molecular Schottky Diodes[1]
PIERRE DARANCET, Argonne Natl Lab — Following early theoretical models [1], efforts towards the synthesis and characterization of more efficient molecular diodes have consisted into attempts to increase the electron rich/poor characters of the donor/acceptor moieties, decrease their conjugation, and imbalance their coupling to the electrodes. The experimental poor performance of single-molecule diodes – with the notable exception of environment-induced diodes [2] – suggests that these physical parameters tend to be mutually exclusive in most molecular systems [3]. In this talk, inspired by recent observations of large rectification ratios at organic bilayers [4], we will show how molecules with a moiety strongly coupled to a metal electrode can, in principle, be used to optimize these different aspects simultaneously. Using first-principles calculations, we will show that this class of molecular systems –analog to macroscopic Schottky diodes, can display large rectification ratios at low operating voltages. [1] Taylor et al. Phys. Rev. Lett. 89, 138301 (2002); Andrews et al. JACS 130, 17309 (2008); [2] Capozzi et al. Nat. Nano 10, 522 (2015); [3] Mujica et al. Chem. Phys. 281, 147 (2002); Stokbro et al. JACS 125, 3674 (2003) ; [4] Smerdon et al., submitted.

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Pierre Darancet
Argonne Natl Lab

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