**Electrochemical potential profiles of molecule junctions using constrained-search density functional study**

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**ABSTRACT**

A reliable first-principles modeling technique for the finite bias-induced non-equilibrium system is highly desired to develop next-generation nano-electronic devices. Although, density functional theory (DFT)-based non-equilibrium Green’s function (NEGF) formalism has been achieved great success in terms of providing insights into novel devices, there still exists a limitation in describing the electrochemical potential, which is a key to interpret the voltage drop in the devices. In this presentation, we show the finite-biased molecule junction systems by applying our recently developed method based on a microcanonical picture that maps steady-state nonequilbrium statistics to drain-to-source excitation named multi-space constrained density functional theory (MS-DFT). We provide their electrical and transport properties and verify our developed formalism as comparing to the DFT-based NEGF method. Moreover, we demonstrate the electrochemical potential profiles and discuss its intrinsic nature in the molecular junctions under a finite bias. This integrated microscopic information will provide the critical insights of the voltage drop in the nano-electronic devices.