A Generalized and Modular Approach to Tunnel-Junction Spectroscopy for Quantum Systems

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We present a generalized and modular scheme for tunneling spectroscopy of 0D quantum systems based on the exfoliation and stacking of 2D heterostructures. In this scheme, layers of graphene/graphite (gr) and hexagonal boronitride (hBN) are assembled into a gr/hBN/hBN/gr tunnel junction. The differential conductance (dI/dV) of this structure is sensitive to both direct tunneling through the insulating hBN and resonant tunneling through any impurity states within the bandgap. As a proof of principle, we demonstrate the ability to resolve a variety of structural defects in hBN as well as the direct observation of the HOMO and LUMO states of vanadyl pthalocyanine (VOPc) encapsulated at the interior hBN/hBN interface of the heterostructure (Fig. 1). The VOPc tunneling spectra directly correlate with scanning tunneling microscopy (STM) of witness samples and are consistent with density functional theory (DFT) of VOPc. This technique is extensible to a wide variety of 0D systems encapsulated at the hBN/hBN interface, including electrically (or redox) active molecular systems, adatoms, and point defects in 2D materials. This generality and flexibility provides an exciting opportunity for both electronic/structural characterization of these quantum states as well as potential applications in quantum information.



Figure 1. (Top Panel) IV and dI/dV acquired from a graphene/hBN/VOPc/hBN/graphene tunnel junction. Peaks in dI/dV correspond to steps in IV as resonant tunneling through VOPc molecular orbitals is allowed. (**Middle Panel**) Same dI/dV data from Top Panel, but with the direct tunneling background removed by fitting to a polynomial background. There is a clear resonance at -2.1 V representing the VOPc HOMO, and additional structure at positive bias that may correspond to the VOPc LUMO. (**Bottom Panel**) STM based tunneling spectra of a similar structure (graphite/hBN/VOPc) confirming the HOMO and LUMO energies of the VOPc.

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