Recent advances in the theoretical modeling of STM/STS on 2D materials by applying Chen's derivative rules in the BSKAN code

K. Palotas[1,2]

[1]Institute for Solid State Physics and Optics, HUN-REN Wigner Research Center for Physics, Budapest, Hungary
[2]HUN-REN-SZTE Reaction Kinetics and Surface Chemistry Research Group, University of Szeged, Szeged, Hungary

Scanning tunneling microscopy/spectroscopy (STM/STS) are inevitable experimental methods to study the local electronic properties of various material surfaces in high spatial and energetic resolution by employing an atomically sharp probe tip.In the first part of the talk I present a new development in the BSKAN code [1] for STM/STS calculations based on first-principles electronic structure data. Recently, we implemented the revised Chen's derivative rules for electron tunneling [2] to enable computationally efficient calculations of the differential conductance dI/dV for STS simulations [3]. By taking pristine and boron- or nitrogen-doped graphene sheets as sample surfaces, the reliability of our implementation is demonstrated by comparing its results to those obtained by the Tersoff-Hamann and Bardeen's electron tunneling models. It is highlighted that the energy-resolved direct and interference contributions to dI/dV arising from the tip's electron orbitals result in a fingerprint of the particular combined surface-tip system. The significant difference between the electron acceptor boron and donor nitrogen dopants in graphene is reflected in their dI/dV fingerprints. The presented theoretical method allows for an unprecedented physical understanding of the electron tunneling process in terms of tip-orbital-resolved energy-dependent dI/dV maps that is anticipated to be extremely useful for investigating the local electronic properties of novel material surfaces in the future.In the second part of the talk I highlight recent important findings applying the BSKAN STM/STS simulation code to a variety of surfaces of current interest: (i) atomic-scale identification of nitrogen dopants in corrugated graphene [4], (ii) electron orbital insights to the effect of CO-functionalized tips in STM [5], (iii) demonstrated element-specific STM imaging of ultrathin copper oxide films [6], (iv) higher-indexed Moire patterns of electronic origin in MoTe2/graphene heterostructures [7], and (v) the STM signatures of stacked charge-density waves in 2H-NbSe2 bilayers [8].

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