3D-WKB-STM

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The 3D-WKB-STM code [1] allows the calculation of (spin-polarized) scanning tunneling microscopy [2] & spectroscopy [3] (STM & STS), i.e., bias-voltage-(V-)dependent tunneling current (I) and differential conductance (dI/dV) in a vacuum tunnel junction based on electronic structure data of the sample surface and the STM tip obtained from first principles. Calculation of a large variety of STM & STS modes is available corresponding to relevant experimental modes, e.g., high-resolution STM images and STS spectra at constant height or constant current, line scans, single point spectra, differential magnetic mode (topographic and magnetic signals).
The theoretical model relies on the orbital-dependent atom-superposition approach of elastic tunneling [4], i.e., contributions from individual electron tunneling transitions between the tip apex atom and each of the sample surface atoms are superimposed assuming the one-dimensional Wentzel–Kramers–Brillouin (WKB) approximation using a geometrically modified transmission function depending on the real space electron orbitals involved in all these transitions. Since the three-dimensional geometry of the tunnel junction is considered, the method is, in effect, a 3D-WKB atom-superposition approach. The electronic structure of the surface and the tip is included in the model by the atom-projected electron density of states (PDOS) that can routinely be obtained by *any* ab initio electronic structure code. So far PDOS produced by VASP, SKKR, FLEUR and SIESTA codes have been used.
The 3D-WKB-STM code is computationally very efficient [1], and it is extremely suitable to investigate tip-related effects on the electron tunneling transport, e.g. on the STM contrast changes [2,4,5,6]. Three unique features include:
1. The ability to calculate bias-voltage-dependent spin-polarized electron transport (STM & STS) above surfaces exhibiting a complex noncollinear magnetic structure [2,3], i.e., without a global spin quantization axis, including the electronic structure of a magnetic tip, at very low computational cost.
2. The ability to investigate tip geometry effects on the STM & STS by considering asymmetric relative tip-sample orientations within the orbital-dependent tunneling [5], which is otherwise computationally very demanding to do.
3. The ability to calculate a statistically large number of relative tip-sample orientations in order to gain insight to the tip geometry in real STM experiments [7].
The usage of the 3D-WKB-STM code has provided important explanations of experimental STM data [5,7,8], and in the future it is continuously expected to be very useful to explore subtle electron transport features observed in STM experiments where strong tip effects play a crucial role that cannot be explained by the simple Tersoff-Hamann model.
The 3D-WKB-STM code is free of charge, and interested users are encouraged to contact K. Palotás directly by email (palotas@phy.bme.hu) to get access to the code.
http://www.phy.bme.hu/~palotas/

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