Topographical fingerprints of many-body interference blocking in STM junctions on thin insulating films

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Negative differential conductance is a nonlinear transport phenomenon ubiquitous in molecular nanojunctions [1]. Its physical origin can be the most diverse. In rotationally symmetric molecules with orbitally degenerate many-body states it can be ascribed to interference effects [2,3,4]. We establish in this paper [5] a criterion to identify the interference blocking scenario by correlating the spectral and the topographical information achievable in a scanning tunneling microscopy (STM) single-molecule measurement. Simulations of current-voltage characteristics as well as constant-height and constant-current STM images (see figures below) for a Cu-phthalocyanine on a thin insulating film are presented as experimentally relevant examples.

References

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Figures

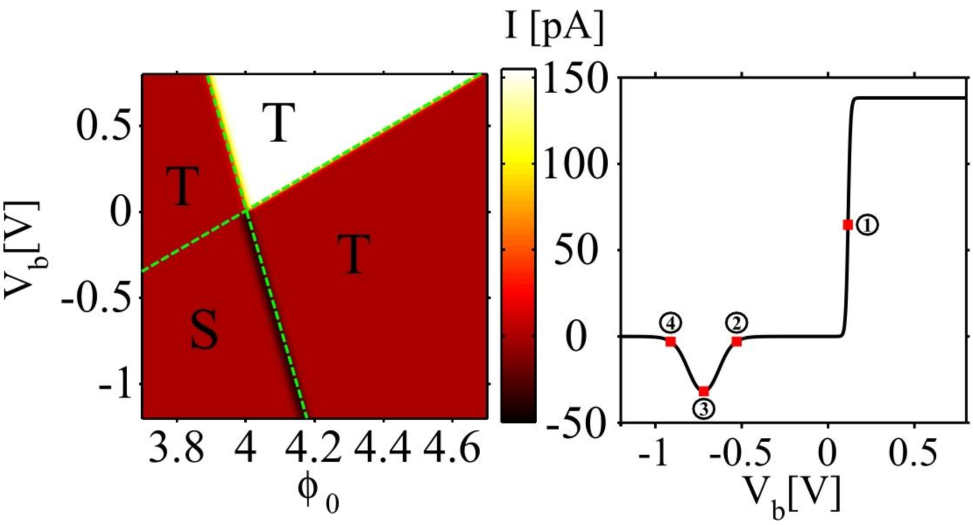

Fig. 1: Left: Current through a CuPc singlemolecule junction as a function of the substrate (and tip) work function φ_0 and of the sample bias V_b Right: Current obtained from a cut of the left-hand plot corresponding to $\varphi_0 = 4.1$ eV. The current scale is the same for the left and right panels. The numbers in the current-voltage plot refer to the current maps in Fig. 2 and Fig. 3.

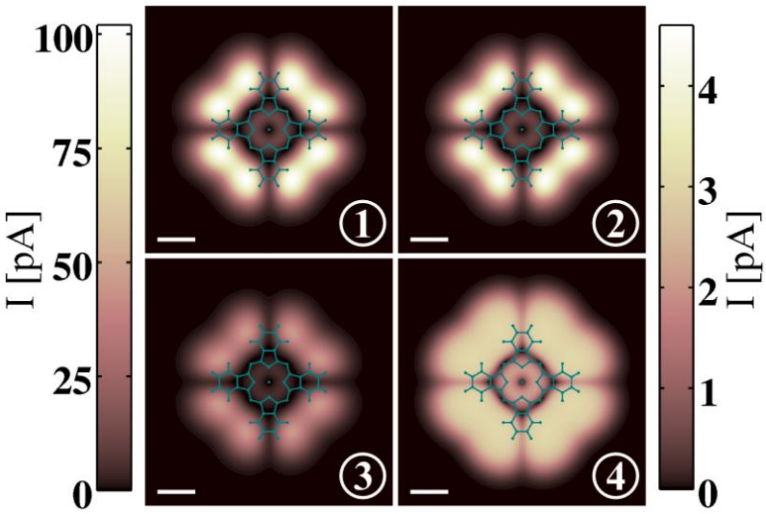

Fig. 2 Constant-height current maps calculated for different bias voltages. The color bar on the left (right)-hand side corresponds to maps 1 and 3 (maps 2 and 4). The current map in the interference blockade regime (map 4) appears to be flat in the molecule region.

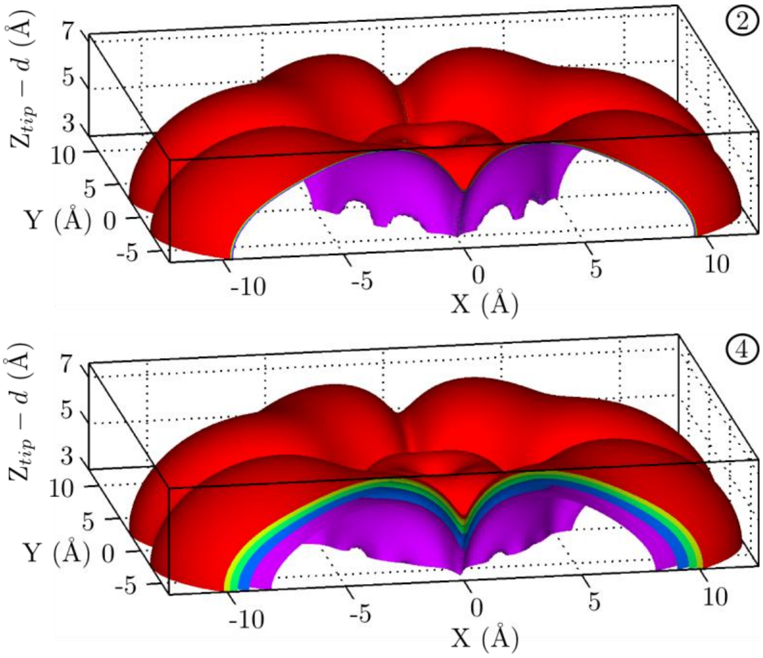

Fig. 3 Isosurfaces of constant current calculated in the proximity of the Coulomb blockade (upper panel; $V_b = 0.5303$ V) and nterference blockade (lower panel; $V_b = -0.9118$ V) regimes. The surfaces correspond, in both cases, to the currents: $I = 3.15$, 3.075, 3.0, 2.925, and 2.85 pA.