Scanning tunneling microscopy simulations based on the revised Chen's derivative rules

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Chen's derivative rules for electron tunneling are revised [1] for the purpose of computationally efficient simulations of scanning tunneling microscopy (STM). The new features include (i) the weighting of tunneling matrix elements of different tip-orbital characters by an arbitrary energy-independent choice or based on first-principles data, (ii) arbitrary tip geometrical orientations enabling the consideration of asymmetric tips, and (iii) the possibility of quantitative analysis of tip-orbital interference contributions to the tunneling current. The model has initially been applied to two functionalized surfaces where quantum interference effects play an important role in the STM imaging and the Tersoff-Hamann model fails to describe the correct STM contrast under certain conditions: N-doped graphene [2] and a magnetic Mn_2H complex on the Ag(111) surface [3]. For both of these surface structures, the importance of interference between s and p_z tip orbit als is highlighted that cause a significant contrast change in the STM images [1]. Moreover, the revised Chen's method has recently been applied (i) to validate a newly proposed structural model for the magnetite Fe_3O_4(110) surface with two-fold oxygen vacancies [4], (ii) to study surface defects in the organic perovskite $CH_3NH_3PbBr_3$ [5], and (iii) to investigate ultrathin Mo-oxide structures on Au(111) [6].

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