Revised Chen's derivative rules for efficient simulations of STM: Recent results on surface oxides

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Advanced simulation tools of scanning tunneling microscopy (STM) are vital for the proper understanding of various physical and chemical processes at material surfaces. For this reason Chen's derivative rules for electron tunneling has been revised [1] to build a computationally efficient STM simulation tool, based on ab-initio electronic structure. This STM simulation method enables (i) the weighting of tunneling matrix elements of arbitrary model tip-orbital compositions, or those directly obtained from density functional theory (DFT) calculations, (ii) arbitrary tip geometrical orientations to mimic asymmetric tip-sample relations, and (iii) a quantitative analysis of direct and interference contributions of the tip orbitals to the electron tunneling current. Recently, this method has been applied to diverse ultrathin complex surface oxides on metal substrates [2–4], where a better agreement with STM experiments has been achieved than obtained with the Tersoff-Hamann (spherical tip orbital) model (see Figure for the "44" O/Cu structure, reproduced from Ref. [4]).

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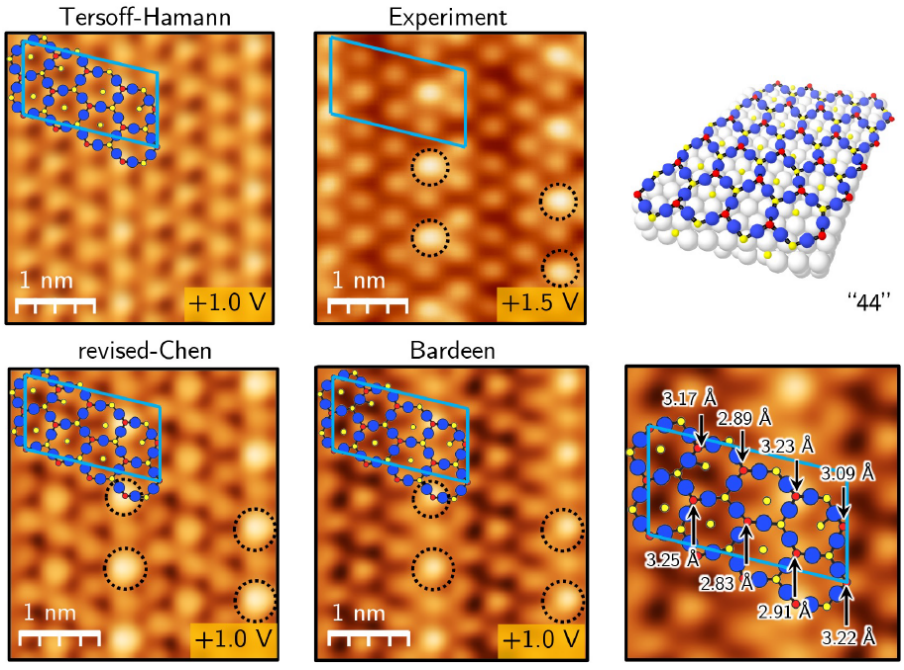

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