

Step edges on galena (100): Probing the basis for defect driven surface reactivity at the atomic scale

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ABSTRACT

Scanning tunneling microscopy (STM) images of the PbS (100) surface with a step and several kinks were obtained with atomic resolution. These images show an increased tunneling current at step edge sites and an apparent deformation of the lattice near the step. The experimental images are compared with theoretical ab initio calculations for which we developed a hybrid method of constant current and constant height mode STM image simulation. With these calculations, we find that the apparent deformation is mainly an electronic effect rather than relaxation of atoms. In addition, with the help of these calculations, we can identify the changes of individual terrace-like and step-like orbitals that are observed using the STM in terms of the energy, density and shape of these states. This detailed knowledge of the electronic behavior of the PbS surface near a step can be used as a basis for explaining adsorption, acid/base, and redox behavior on PbS terraces and at steps, and the differences between the two.