Surface Defects on Cu(111): A combined STM & DFT study

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The (111) termination of copper is an important substrate for the growth of promising two-dimensional materials and thin-films, such as graphene [1] and cerium oxide [2]. Surface defects can play an important role in the growth and properties of these materials. Moreover, the study of surface defects is of importance to Scanning Tunnelling Microscopy (STM) and surface science research, as high resolution atomic-scale features can reveal interesting atomic-scale phenomena. For these reasons, we have performed a combined STM and Density Functional Theory (DFT) investigation of Cu(111) surface defects.

Two defects are of particular interest. Firstly, a dipole-like feature contained within a hexagonal defect to the Cu(111) lattice. Secondly, a bright hexagonal ring encompassing a dark atom-sized defect. Initial DFT calculations, performed within the Quantum Espresso code [3], indicate that these features are due to non-copper atoms residing in defects of the Cu(111) lattice. In the case of the bright hexagonal ring, hydrogen is suggested to reside in the defect site. Finally, nearby (off the order of several nanometers) bright hexagonal rings have been observed to interact with each other.

References:
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