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Gold on silicon: Can theory and experiments for Si(111)-(5x2)-Au be reconciled? STEVEN ERWIN, Naval Research Laboratory, CHRISTOPH SEIFERT, Universität Duisburg-Essen, Duisburg, Germany — Since its discovery 30 years ago, the 5x2 reconstruction of Si(111) induced by 2/5 monolayer of Au has been widely studied for its unusual one-dimensional electronic properties. Despite quite detailed and consistent data from a variety of surface science techniques, there is still no structural model consistent with the constraints inferred from those data. Here we combine density-functional theory (DFT) and scanning tunneling microscopy (STM) data to systematically develop and investigate new candidate structural models. The underlying 5x2 parent reconstruction is decorated by Si adatoms, whose density is at most one adatom per two 5x2 unit cells, and at equilibrium is half of this limit. We consider first the adatom-free parent reconstruction. Starting from simple principles of dangling bonds and surface stress relief, we construct a well-defined set of chemically plausible models that can be exhaustively generated by combinatorics. Several recently proposed models for Si(111)-(5x2)-Au are examples from this set. We then consider the role of the Si adatoms. We find that their role is two-fold: to passivate dangling bonds and to dope the parent band structure. Using the complete model, detailed predictions for STM imagery and surface band structure compare favorably with experiment.

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