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H-induced Magnetism at Stepped Si (100) Surface

Jun-Ho Lee, Jun-Hyung Cho

Department of Physics, Hanyang University

Using spin-polarized density-functional theory calculations, we find that the existence of either Peierls instability or antiferromagnetic spin ordering is sensitive to hydrogen passivation near the step. As hydrogens are covered on the terrace, the dangling bond electrons are localized at the step, leading to step-induced states. We investigate the competition between charge and spin orderings in dangling-bond (DB) wires of increasing lengths fabricated on an H-terminated vicinal Si(001) surface. We find antiferromagnetic (AF) ordering to be energetically much more favorable than charge ordering. The energy preference of AF ordering shrinks in an oscillatory way as the wire length increases. This oscillatory behavior can be interpreted in terms of quantum size effects as the DB electrons fill discrete quantum levels.

Keywords: surface magnetism, Si (100) surface, step edge, hydrogen-induced magnetism, spin-polarized density functional theory, quantum size effect