Theoretical Prediction of Heterogeneous Molecular Wires on the Si(001) Surface

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Using first-principles density-functional calculations, we propose a self-assembly technique for fabrication of the heterogeneous molecular wire on the dangling-bond wire generated on an H-passivated Si(001) surface. Here, we choose pyridine and borine as Lewis base and acid molecules, respectively, to demonstrate different behaviors in the chemical reactivity and selectivity on the dangling-bond wire, leading to formation of the heterogeneous pyridine-borine wire. Additionally we present of the Peierls instability in the 1D borine wire formed on the Si(001) surface. We find that this molecular wire is stabilized by formation of a 1D-CDW, accompanying a structural distortion with a double periodicity and a band-gap opening at the Fermi level. Such a 1D molecular wire on the 2D substrate may provide a model system to allow a real-space observation of CDWs, their fluctuations or critical behaviors at atomic scale.