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An Ab Initio Study of Hydrogenation induced Metallization of SiC001 (3x2)

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Abstract:

We will present results for the band structure of hydrogenated Silicone Carbide (001) (3x2) surface with various levels of hydrogenation. These band structures were obtained using density functional theory with a generalized gradient exchange correlation function. Further, the calculations reveal the following scenario. Initially, Hydrogen atoms saturate all the dangling bonds of the surface dimers. This in turns allows for the subsequent H atoms to bind with Si atoms in the second layer. Those new bonds for the appropriately hydrogenated surface cause a “metallization" of the surface. Hydrogenation beyond that brings the system to its semiconducting state.