Electronic properties of Si-C interfaces

Xiang-Guo Li, Hai-Ping Cheng, Department of Physics, University of Florida, USA — In this work, we report our investigations of interfacial properties of Si-C systems. Electronic properties of Fe-doped carbon on silicon surfaces, Si-Fe-C layered structures and Si-graphene-Si junctions have been studied using first-principles calculations. Charge transfer at the interfaces, densities of states, and magnetization are fully analyzed. These problems are important because recent experiments show that Fe@C-Si materials have giant electro-resistance and magneto-resistance highly sensitive to the external magnetic field. The non-magnetic feature leads to very small magnetic noise. In addition, photovoltaic effects were also observed in some of these systems.

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