

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

An ab initio study of the interaction of transition metal atoms with single-wall armchair SiC nanotubes¹ KAZI ALAM, ASOK RAY — A systematic study of Fe atom encapsulated and adsorbed in armchair SiC nanotubes has been performed using hybrid density functional theory calculations within finite cluster approximation. A detailed comparison of the binding energies, equilibrium positions, Mulliken charges and spin magnetic moments of Fe atoms has been performed for three types of nanotubes. The electronic states, HOMO-LUMO gaps, and changes in gaps with respect to the bare nanotube gaps have been investigated as well. Binding energies of the encapsulated and adsorbed Fe atoms indicate that these structures are stable and show site dependence. For both cases significant band gap decrease is observed for type 1 nanotubes enabling band gap tailoring. This decrease is not observed for the other two types in both cases of interactions. All the structures are found to have magnetic ground states with very high magnetic moments indicating the possibility of them being used as nanomagnets.

¹This work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525)

Kazi Alam

Date submitted: 21 Nov 2007

Electronic form version 1.4