Electronic Supplementary Information

Improved Binding and Stability in Si/CNT Hybrid Nanostructures via Interfacial Functionalization: a First-Principles Study

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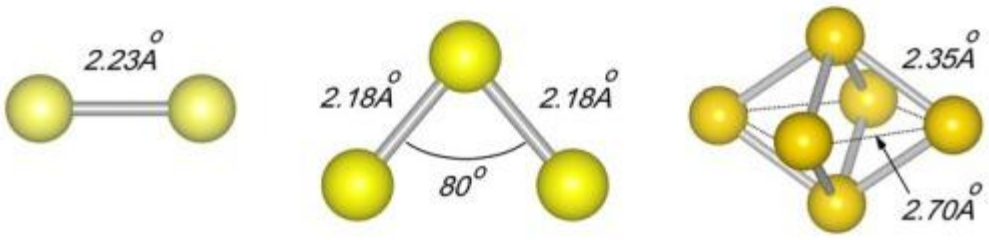

Figure S1. Initial structures of Si2, Si3 and Si6 clusters

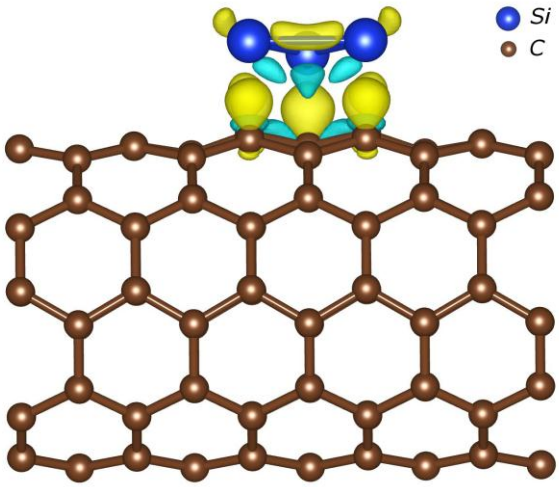

Figure S2. Contour plot of charge-density difference in Si_3/CNT nanostructure (Configuration Si_3-Par). Yellow color indicates positive regions (charge accumulation), while blue – negative (charge depletion)

The transferred electrons are mainly accumulated at the region of Si-C bonds. Note the charge accumulation on Si-Si bond, which is newly formed when Si_3 changed its shape from isosceles to equilateral triangle.