Lowdimensional Nanostructures
Assignment 1

January 13, 2010

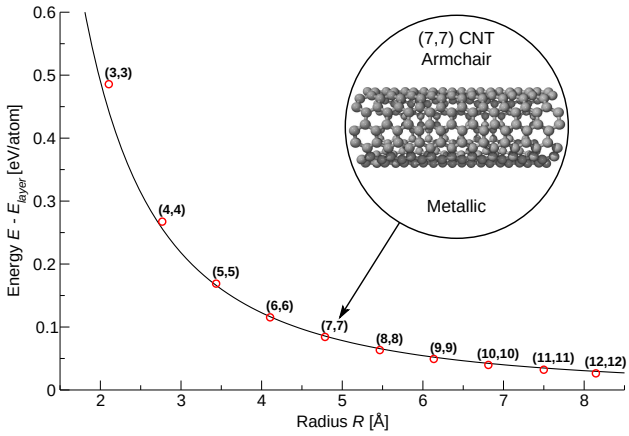

Figure 1: Formation energy $\Delta E_{\rm form} = E_{\rm SWNT} - E_{\rm graphene}$ per C atom in a single-walled carbon nanotube (SWNT) relative to graphene

Q1. The formation energy $\Delta E_{\rm form} = E_{\rm SWNT} - E_{\rm graphene}$ per C atom in a single-walled carbon nanotube (SWNT) relative to graphene may be expressed as a function of the nanotube radius R, as shown in Fig. 1. Derive an expression to leading order for $\Delta E_{\rm form}$ in terms of the SWNT radius.

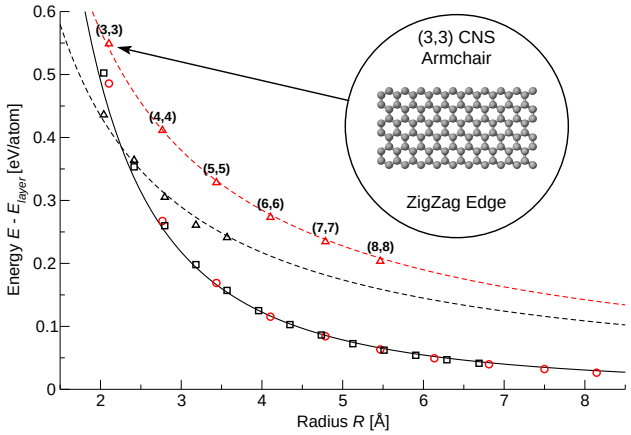

Figure 2: Formation energy $\Delta E_{\rm form} = E_{\rm NR} - E_{\rm graphene}$ per atom in a carbon nanoribbon (NR) relative to graphene

Q2. The formation energy $\Delta E_{\rm form} = E_{\rm TiO_2NR} - E_{\rm TiO_2}$ per TiO_2 functional unit in a carbon nanoribbon (NR) relative to the infinite graphene layer may also be expressed as a function of the nanoribbon's width R, as shown in Fig. 2. Derive an expression to leading order for $\Delta E_{\rm form}$ in terms of the nanoribbon's width in eV/C.

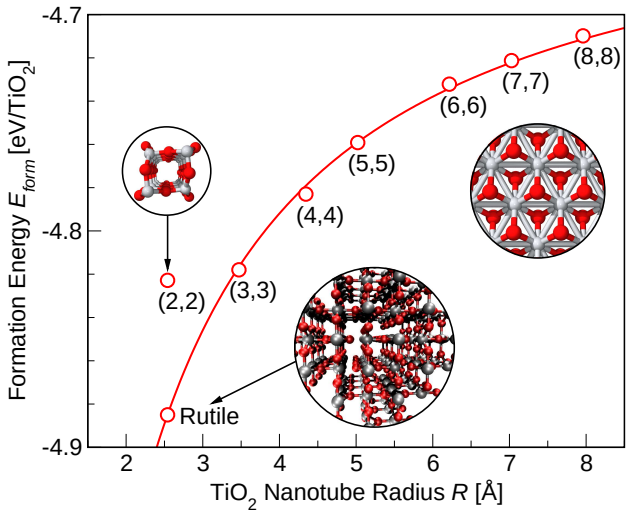

Figure 3: Formation energy $\Delta E_{\rm form} = E_{\rm TiO_2NT}$ per atom in a TiO_2 nanotube (TiO_2NT) relative to a TiO_2 functional unit.

3. The formation energy $\Delta E_{\rm form} = E_{\rm TiO_2NT} - E_{\rm TiO_2}$ per TiO_2 functional unit (TiO_2 NT) relative to a TiO_2 functional unit may also be expressed as a function of the nanotube's radius R, as shown in Fig. 3. Derive an expression to leading order for $\Delta E_{\rm form}$ in terms of the nanotube radius, the TiO_2 layer energy, and the rutile TiO_2 bulk's energy, in eV/TiO_2.