Quantum Size Effect in Ag Nanoclusters – Carbon Nanotubes Interfaces

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The electronic properties of interfaces made of metallic or semiconducting carbon nanotubes (CNT) and icosahedral Ag nanoclusters (AgNC) containing 13 and 55 atoms were studied with the help of DFT calculations [1]. Using suitable supercell geometries managed with the python module [2], we are showing that the Ag nanocluster size has a strong influence on the magnitude of the charge transfer (see Figure 1(b)), on the wave function evanescence into the CNT and on the local dipole at the vicinity of the AgNC-CNT interface. The electronic properties of the Ag-CNT interface can be partly controlled through the adsorption of gas such as CO on the Ag surface clusters which modulates the adsorption energy and the magnitude of the charge transfer as seen in figure 1(b). Similar analyses were performed for a CNT-AgNC-CNT junction (see Figure 2).

References

[1] Soler, J. M., Artacho, E., Gale, J. D., García, A., Junquera, J., Ordejón, P., & Sánchez-Portal, D. *Journal of Physics: Condensed Matter*, 14, (2002), 2745–2779

[2] Hjorth Larsen, A., Jørgen Mortensen, J., Blomqvist, J., Castelli, I. E., Christensen, R., Dułak, M., Jacobsen, K. W., *Journal of Physics: Condensed Matter*, 29, (2017), 273002 (30pp)

Figures

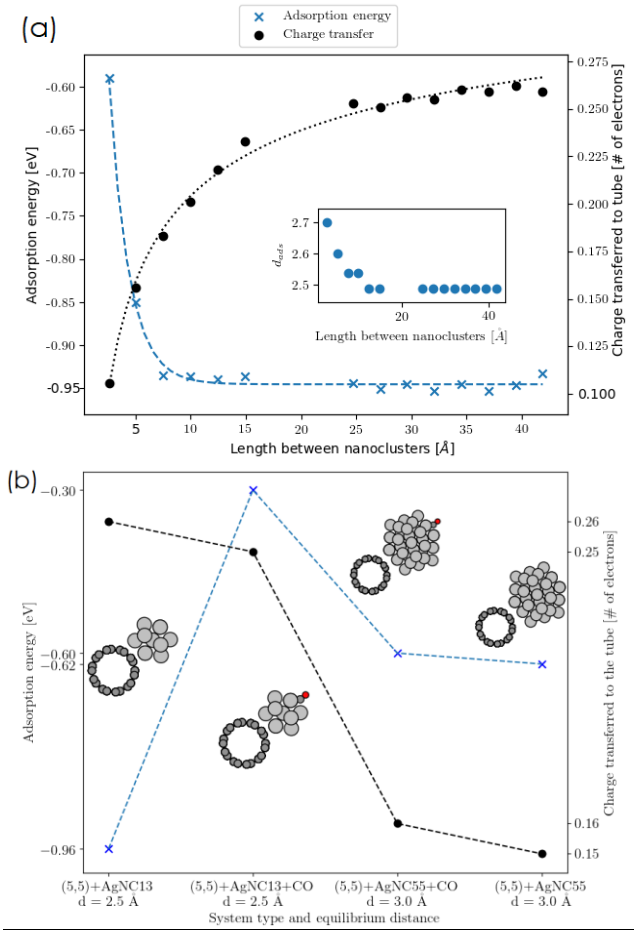

Figure 1: (a) The variation of charge transfer and adsorption energy of a AgNC13 on a zigzag (5,5) CNT as a function of the distance separating the cluster from it's periodic image. The inset shows the variation of the equilibrium distance. (b) Calculated properties of the (5,5) CNT with several cluster types. The legend in (a) applies to both subfigures. The lines are guides.

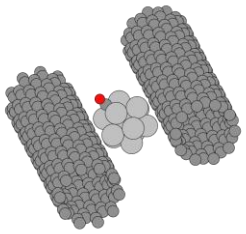

Figure 2: Considered geometry for realistic junction made of two (10,0) nanotubes and a AgNC with an adsorbed CO molecule