Realistic modeling of carbon nanostructures, bridging the gap between theory and experiment

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Abstract

Computer simulation has played a determinant role in the explosive development of carbon nanotechnology by predicting and explaining novel electronic properties in carbon nanomaterials. In recent years (and in a more modest scale) we have used and developed different quantum chemical models to explain complex experimental results involving the electronic structure of fullerenes, carbon nanotubes and graphite. We will show how experimental data can be accounted by different models with up to thousands of atoms [1-3]. We will also present and discuss cases where accurate dispersion is fundamental, from the, fundamental, *intermolecular* binding in graphite and fullerene crystals to the curling of graphene in solution [4] and the encapsulation of molecules in nanotubes [5].

References

[1] P. Ruffieux, M. Melle-Franco et al. PRB, **15** (2005) 153403.
[2] M. Melle-Franco, M. Marcaccio, D. Paolucci, et al. JACS, **6**, (2004) 1646.
[3] D. Paolucci, M. Melle Franco et al. JACS, **23** (2008):739.
[4] A. Catheline, L Ortolani, V Morandi, M. Melle-Franco, C. Drummond, C. Zakri and A. Pénicaud, Soft Matter, **8** (2012) 7882.
[5] TW. Chamberlain , RF. Pfeiffer , J. Howells , H. Peterlik , H. Kuzmany , B. Kräutler , T. Da Ros , M. Melle-Franco , F. Zerbetto , D. Milićand and AN. Khlobystov, Nanoscale, **4** (2012) 7540.

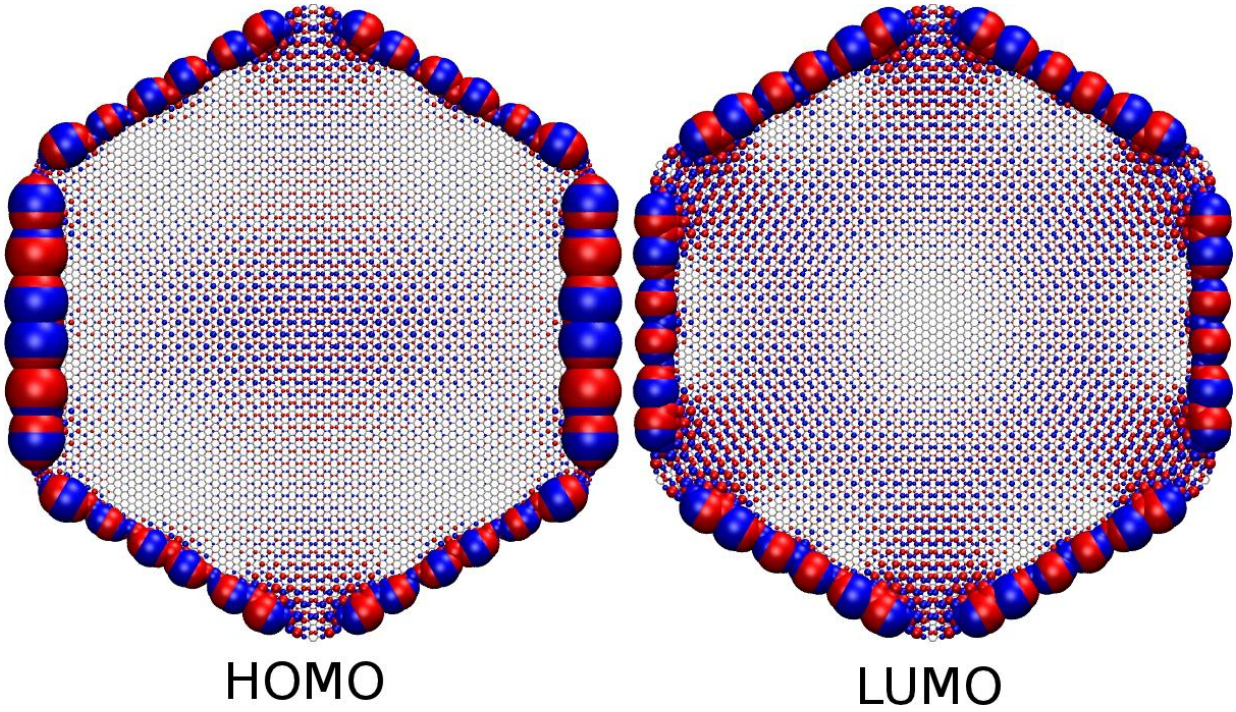

Figure 1. Frontier orbitals of graphene island with Zig-Zag borders and 9600 carbon atoms calculated with a multiscale tight binding model.