

Conferencia:

How to use Computational Chemistry to understand experiments in Carbon Nanomaterials

Manuel Melle Franco

Departamento de Química,
CICECO, Universidade de Aveiro,
Aveiro, Portugal

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How to use Computational Chemistry to understand experiments in Carbon Nanomaterials

Manuel Melle-Franco

Departamento de Química, CICECO, Universidade de Aveiro, Aveiro, Portugal.

manuelmelle.research@gmail.com

Computer modelling has become a fundamental tool to understand and rationalize new molecules and materials. Through the years we have applied and developed several computational models to explain different experiments on carbon-based materials and molecules. We will show, from the experimental point of view and in a fully non-technically manner, several examples of our work where models complemented and completed experimental science. Nanomaterials ranging from polydisperse carbon nanomaterials like functionalized carbon nanotubes [1] to monodisperse, novel, bottom-up materials [2-4] will be presented.

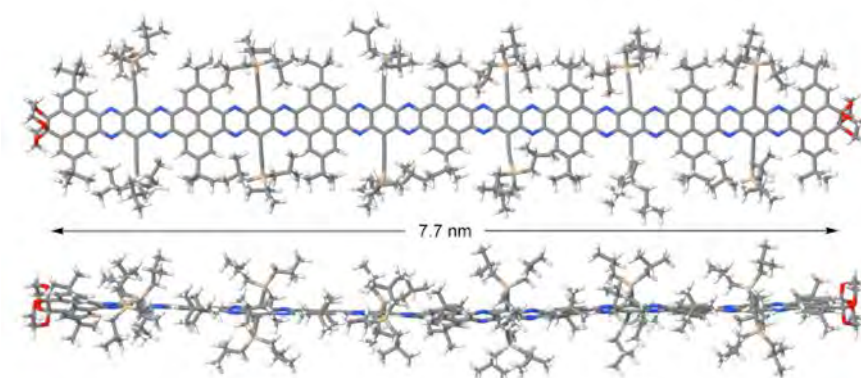


Figure 1. Soluble monodisperse graphene nanoribbon from synthetic chemistry [2].

[1]^aManuel Melle-Franco, Massimo Marcaccio, Demis Paolucci, Francesco Paolucci, Vasilios Georgakilas, Dirk M. Guldi, Maurizio Prato, and Francesco Zerbetto, *Journal of the American Chemical Society*, 2004, 126, 1646.^bPaolucci, Demis, Manuel Melle Franco, Matteo Iurlo, Massimo Marcaccio, Maurizio Prato, Francesco Zerbetto, Alain Pénicaud, and Francesco Paolucci, *Journal of the American Chemical Society*, 2008, 130, 7393. ^cSalvador, Andreia F., Gilberto Martins, Manuel Melle-Franco, Ricardo Serpa, Alfons J.M. Stams, Ana J. Cavaleiro, M. Alcina Pereira, and M. Madalena Alves, *Environmental Microbiology*, 2017, 19, 2727.

[2] Cortizo-Lacalle Diego, Mora-Fuentes Juan P., Strutyński Karol, Saeki Akinori, Melle-Franco Manuel, and Mateo-Alonso Aurelio, *Angewandte Chemie*, 2017, 57, 703.

[3] Marco A. Belen, Cortizo-Lacalle Diego, Perez-Miqueo Iñigo, Valenti Giovanni, Boni Alessandro, Plas Jan, Strutyński Karol, et al. *Angewandte Chemie*, 2017, 129, 7050–55.

[4] Carini, Marco, Marta P. Ruiz, Imanol Usabiaga, José A. Fernández, Emilio J. Cocinero, Manuel Melle-Franco, Ismael Díez-Perez, and Aurelio Mateo-Alonso, *Nature Communications*, 2017, 8, 15195.

Manuel Melle-Franco - Short CV 15/05/2018



Manuel Melle-Franco was born in Lugo (Spain) in 1972 and has a 5 year degree in Physical-Chemistry from University of Santiago de Compostela (Spain) and an M.Sc. in Materials Chemistry from University of Kent (UK), where he later pursued his Ph.D.

Manuel worked one year in the Materials Department of University of Milano-Bicocca (Italy) with Gianfranco Pacchioni and got his Ph.D. in Chemical Physics with Alan Chadwick from University of Kent (UK) in 2001. After that, he worked with Francesco Zerbetto in the department of Chemistry of University of Bologna (Italy) for 8 years, and later he moved to Portugal, where he worked as an independent researcher in University of Porto and University of Minho, before joining CICECO - Aveiro Institute of Materials, in University of Aveiro in 2016.

Manuel currently leads the **Applied Computer Modelling Group @ CICECO** which applies several atomistic computational techniques to interesting experimental problems in chemistry, biochemistry, materials chemistry and physics. Manuel's main research line is carbon-based nanomaterials, like **carbon nanotubes, graphene, fullerenes, nanoribbons, nanohorns**, etc. Manuel has currently 60 publications, of which 35% as first/corresponding author, with an **added impact factor of 345**.

Selected publications (click for links!)

1. Cortizo-Lacalle, Diego, Juan Pedro Mora-Fuentes, Karol Strutyński, Akinori Saeki, Manuel Melle-Franco*, and Aurelio Mateo-Alonso. "Monodisperse N-Doped Graphene Nanoribbons Reaching 7.7 Nm in Length." *Angewandte Chemie International Edition*, In-press. doi:10.1002/anie.201710467. IF=11.7.
2. Carini, Marco, Marta P. Ruiz, Imanol Usabiaga, José A. Fernández, Emilio J. Cocinero, Manuel Melle-Franco, Ismael Díez-Pérez, and Aurelio Mateo-Alonso. "High Conductance Values in π -Folded Molecular Junctions." *Nature Communications* 8 (May 18, 2017): 15195. doi:10.1038/ncomms15195. IF=11.3.
3. Marco, A. Belen, Diego Cortizo-Lacalle, Iñigo Perez-Miqueo, Giovanni Valenti, Alessandro Boni, Jan Plas, Karol Strutyński, et al. "Twisted Aromatic Frameworks: Readily Exfoliable and Solution-Processable Two-Dimensional Conjugated Microporous Polymers." *Angewandte Chemie International Edition*, January 1, 2017, in-press. doi:10.1002/anie.201700271. IF=11.7.
4. Melle-Franco, Manuel. "Graphene Fragments: When 1 + 1 Is Odd." *Nature Nanotechnology* advance online publication (February 13, 2017). doi:10.1038/nnano.2017.9. IF=35.3.
5. Dallavalle, M., Calvaresi, M., Bottoni, A., Melle-Franco, M., Zerbetto, F., "Graphene Can Wreak Havoc with Cell Membranes" *ACS Applied Materials & Interfaces* 7, no. 7 (February 25, 2015): 4406–14, doi:10.1021/am508938u. IF=6.72.
6. Melle-Franco, M., "Uthrene, a Radically New Molecule?" *Chemical Communications* 51, no. 25 (2015): 5387–90, doi:10.1039/C5CC01276G. IF=6.3.
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9. Paolucci, D., Melle-Franco, M., Iurlo, M., Marcaccio, M., Prato, M., Zerbetto, F., Pénicaud, A., Paolucci, F., "Singling out the Electrochemistry of Individual Single-Walled Carbon Nanotubes in Solution," *Journal of the American Chemical Society* 130, no. 23 (2008): 7393–99, doi:10.1021/ja710625p. IF=12.1.
10. Bellarosa, L., Bakalis, E., Melle-Franco, M., Zerbetto, F., "Interactions in Concentric Carbon Nanotubes: The Radius vs the Chirality Angle Contributions" *Nano Letters* 6, no. 9 (2006): 1950–54, doi:10.1021/nl061066g. IF=13.6.
11. Melle-Franco, M., Zerbetto, F., "Ejection Dynamics of a Simple Liquid from Individual Carbon Nanotube Nozzles" *Nano Letters* 6, no. 5 (May 2006): 969–72, doi:10.1021/nl060154y. IF=13.6.
12. Melle-Franco, M., Marcaccio, M., Paolucci, D., Paolucci, F., Georgakilas, V., Guldi, D.M., "Cyclic Voltammetry and Bulk Electronic Properties of Soluble Carbon Nanotubes" *Journal of the American Chemical Society* 126, no. 6 (2004): 1646–47, doi:10.1021/ja039918r. IF=12.1.