Investigating soft matter self-assembly with computer simulations

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In this talk, some aspects of the self-assembly of organic molecules will be faced from the physical chemistry perspective and on the basis of classical computer simulations results, with the aim of giving a flavor of my recent research activity.
The presentation will be divided in four brief sections:

1) An *introduction on molecular and atomistic simulations*, including the description of the selection of the model and the choice and the calculation of its parameters.

2) *Phase behavior of liquid crystals*[1]: the united atom force field for alkyl-cyano biphenyls will be described with regard to the comparison of its performance with experimental results and an outlook on its recent applications.

3) *Magnets on a surface*[2]: the self-assembling process and the aggregate characterization of Tb-phthalocyanine double decker complexes on highly oriented pyrolitic graphite will be presented, also considering their single-molecule magnets characteristics.

4) *Organic crystal growth*[3]: the results of a simulation study of the vapor growth of pentacene on the C_{60} (001) surface will be shown, with the two-fold purpose of understanding the growth process and its final result, and of demonstrating the possibility of reproducing it with computer simulations.

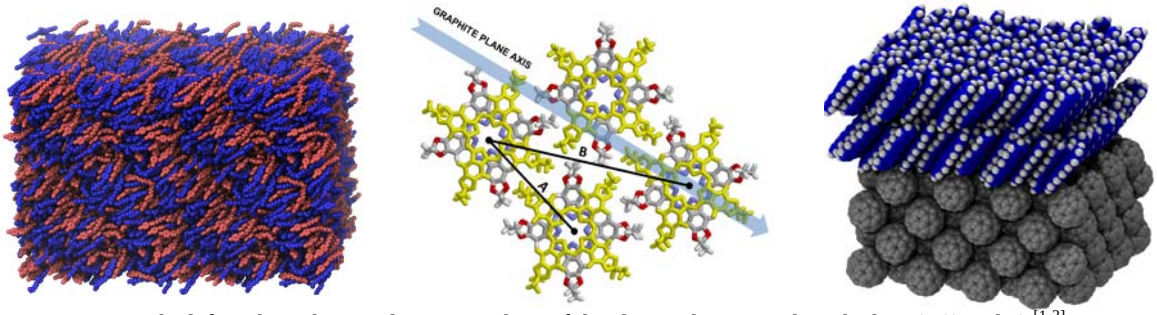

Figure: From the left to the right, simulation snapshots of the chemical systems described in 2), 3) and 4) [1-3].

[1] G. Tiberio, L. Muccioli, R. Berardi, C. Zannoni, *"Towards in silico liquid crystals. Realistic transition temperatures and physical properties for n-cyanobiphenyls via molecular dynamics simulations"*, ChemPhysChem 10, 125-136 (2009), M. F. Palermo, A. Pizzirusso, L. Muccioli, C. Zannoni, *"An atomistic description of the nematic and smectic phases of 8CB"*, in preparation (2011)
[2] M. Gonidec, R. Biagi, V. Corradini, F. Moro, V. De Renzi, U. del Pennino, D. Summa, L. Muccioli, C. Zannoni, D. B. Amabilino, J. Veciana, *"Surface supramolecular organization of a terbium (III) double-decker complex on graphite and its single molecule magnet behavior"*, J. Am. Chem. Soc., 133, 6603-6612 (2011)
[3] L. Muccioli, G. D'Avino, C. Zannoni, *"Simulation of vapor-phase deposition and growth of a pentacene thin film on C60 (001)"*, Adv. Mater., in press, (2011), DOI: 10.1002/adma.201101652