Séminaire de Chimie Théorique

Salle conference ISM 3eme Est, Bat. A12
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Simulating molecular organisations of liquid crystals and other functional materials in the bulk and close to interfaces

Many practical applications of liquid crystals (LC) and organic semiconductors, as well as many fundamental physics problems deal with molecular organizations close to interfaces [1]. Here we plan to show results for the simulation of these organizations at molecular and atomistic resolution. While molecular resolution models have an important role in studying trends and simple devices [2], atomistic molecular dynamics simulations [3] can in principle predict actual morphologies and properties at various temperatures and working conditions from a specific molecular structure. In the talk we present some recent examples of atomistic simulations for various systems [4-6] trying to show the range and applicability of the results for liquid crystals and organic electronics.

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[2] M. Ricci, M. Mazzeo, R. Berardi, P. Pasini and C. Zannoni, A molecular level simulation of a Twisted Nematic cell, *Faraday Discuss.* 144, 171 (2010)
[3] G. Tiberio, L. Muccioli, R. Berardi and C. Zannoni , Towards in silico liquid crystals. Realistic transition temperatures and physical properties for n-cyanobiphenyls via molecular dynamics simulations, *ChemPhysChem* 10, 125 (2009)
[4] A. Pizzirusso, L. Muccioli , M. Ricci and C. Zannoni , Predicting surface anchoring: molecular organization across a thin film of 5CB liquid crystal on silicon, *Chem. Sci.*, published on line (2011)
[5]T.A. Papadopoulos, L. Muccioli, S. Athanasopoulos, A.B. Walker, C. Zannoni, D. Beljonne, Does supramolecular ordering influence exciton transport in conjugated systems? Insight from atomistic simulations, *Chem. Sci.*, **2**, 1025-32 (2011)
[6] L. Muccioli, G. D'Avino and C. Zannoni , Simulation of vapor-phase deposition and growth of a pentacene thin film on C60(001), *Adv. Mater.* **23**, 4532-6 (2011)

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