ON THE DESCRIPTION OF WET, BIO AND NANO SYSTEMS WITH LINEAR-SCALING DENSITY-FUNCTIONAL THEORY

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The efficiency of present-day density-functional theory (DFT) calculations, together with the ever increasing power of modern computers, opens first-principles calculations to sizes and complexities that used to be the realm of empirical calculations only. Problems in wet sciences (wet chemistry, biochemistry, geochemistry, environmental sciences) and nano sciences appear amenable to first-principles approaches, and these simulations are acquiring an increasing presence in those fields. These simulations, however, force us to face more challenges than just size. On the one hand, *complexity*, from the point of view of the nuclear degrees of freedom: wet science demands finite temperature simulations, and thus statistical sampling. First-principles molecular dynamics (FPMD) has become the most popular way (albeit demanding) of attacking such difficulties. On the other hand, *accuracy:* most processes in wet systems depend crucially on interactions as weak as the Van der Waals forces. These represent a hard problem to address: although there are well-established methods in quantum chemistry to address dispersion interactions, they are heavier than DFT methods, and still not practical for FPMD simulations.

After a brief introduction to efficient linear-scaling DFT [1], I will review the situation for using it as a basis for FPMD simulations of water [2-4], concentrating on the effects of accuracy in the properties of the liquid, and on recent efforts to overcome DFT's weaknesses with dispersion interactions. Complementing it with applications relevant to nanobio, recent results will be presented on the nano-bio-wire given by the pilin protein obtained from the pili issued by the geobacter sulfurreducens bacteria in order to feed from electrons at a distance [5].

References:

[1] J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón, and D. Sánchez-Portal, J. Phys. Condens. Matter, **14** (2002) 2745.

[2] M. V. Fernandez-Serra and E. Artacho, J. Chem. Phys. **121** (2004) 11136.

[3] M. V. Fernandez-Serra, G. Ferlat, and E. Artacho, Mol. Sim. **31** (2005) 361.

[4] M. V. Fernandez-Serra and E. Artacho, Phys. Rev. Lett. **96** (2006) 016404.

[5] G. Reguera, K. D. McCarthy, T. Mehta, J. S. Nicoll, M. T. Tuominen, and D. R. Lovley, Nature **435** (2005) 1098.