CIC nanoGUNE
nanoscience cooperative research center

SUMMER INTERNSHIPS 2016

TITLE: Optimising first-principles calculations of matter and nanomattter with supercomputers

DESCRIPTION (Objectives, tasks, materials, equipment…):

Present-day numerical simulation of matter at the nanoscale is done mostly from first-principles, meaning that one starts from the fundamental equations of the theory relevant to the scale (in this case the quantum mechanics of electrons and nuclei) and introduces approximations that render their solution feasible in a realistic time. The most usual approach is based on density functional theory, and present-day DFT programs can deal with up to thousands of atoms in large supercomputers. This project will be dedicated to the testing of basic approximations in the SIESTA program [1,2], a well-known and extensively used DFT code. Most importantly, the basis states in which wave-functions are expanded will be systematized. An adoptive basis idea will be tried which could improve on the efficiency and applicability of quantum-mechanical simulations (Krylov). The project will require the use of supercomputers.

[1] J. M. Soler et al, J. Phys.: Condens. Matter 14, 2745–2779 (2002).
[2] E. Artacho et al, J. Phys.: Condens. Matter 20, 064208 (2008).

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SUITABLE FOR: Physicists and chemists