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SEMINAIRE

energie atomique • energies alternatives

Service de Recherches de Métallurgie Physique

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Salle de réunion du SRMP – Bâtiment 520 – Pièce 109

Computational electronic-structure descriptions of periodic molecular structures : reconciling Gaussians with plane waves

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Electronic-structure calculations based upon density-functional theory (DFT) have become the workhorse of much computational and theoretical research in quantum chemistry and solid-state physics. In the quantum-chemistry community, calculations are most often carried out in the framework of Gaussian-type-orbital (GTO) basis sets for the study of finite nonperiodic molecular assemblies, whereas plane waves (the eigenvectors of the translational-symmetry operators) are preferred for the description of solid-state systems that exhibit full three-dimensional periodicity.

In the intermediate range, i.e., for partially periodic one-dimensional systems (e.g., polymers and nanotubes) and two-dimensional systems (e.g., slabs and single layers), calculations rely on more cumbersome computational strategies, the plane-wave supercell approximation, which consists of extrapolating the physical properties of a system in the limit of large separation between artificial

periodic images, being one of the most popular options.

In this presentation, I will present alternative routes for correcting periodic-image errors that result from the use periodic-boundary conditions for systems that do not exhibit full three-dimensional periodicity. Such computational strategies are based upon multigrid techniques (the real-space countercharge correction) or electrostatic auxiliary functions (the reciprocal-space countercharge correction). The precision of both methods will be shown for a range systems within DFT and hybrid DFT, putting plane-wave calculations on par with refined GTO predictions.

Both real- and reciprocal-space methods are available under the terms of free public licenses.

Mardi 20 septembre 2011 à 10h30

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