SEMINAIRE ISMO

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Modeling Surface-Surface and Molecule-Surface Interactions made «Simple" by Subsystem Density-Functional Theory

In this talk, I will show that a subsystem formulation of DFT can simplify both the theoretical framework and the computational effort for calculating the electronic structure of condensed phase systems. I claim that the naturally subsystem-like form of molecular aggregates (including molecules at surfaces) makes subsystem DFT a better descriptor of the underlying physics than regular DFT of the supersystem. Theory side, I will present a novel van der Waals DFT theory based on subsystem DFT and, thus, theoretically exact and amenable to sensible approximations. Computational side, I will present new implementations of the ground-state theory and the real-time TD-DFT extension of the Frozen Density

Embedding formulation of subsystem DFT in a plane wave basis, I will discuss novel schemes for efficient use of the Brillouin Zone sampling and imposition of spin constraints aided by several pilot calculations which will include molecules at surfaces and layered systems.

Attention ! Jour inhabituel

Jeudi 8 janvier 2015 à 11h
Bât 210 – Amphi 1 (2ème étage)
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