CEA - Saclay 91191 Gif-sur-yvette Cedex

Service de Physique de l'Etat Condensé

SÉMINAIRE

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Mardi 18 novembre 14h00

Orme des Merisiers SPEC Salle Itzykson, Bât.774

Towards density functional theory calculations of defects in crystals

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This talk will describe ongoing work on a method – Quasicontinuum Density Functional Theory – to enable density functional theory calculations of defects in crystals. Defects determine critical properties of crystalline materials even though they occur at relatively low concentrations. They can interact over long distances through slowly decaying fields whose strength depends on the electronic structure of the core. Thus the study of defects requires electronic resolutions with continuum range. The main idea of the current method is a numerical discretization that adapts the resolution to the structure of the solution with no a priori ansatz or ad hoc patches. We demonstrate the idea with Orbital-free Density Functional Theory, highlight key properties through examples and describe ongoing work with DFT.
