

First-principles study of the dielectric response of high permittivity nanocomposites based on perovskites.

The development of new devices for the production and transport of electricity (such as batteries, capacitors, fuel cells, thermoelectricity, photovoltaic, ...) faces new challenges. The principal one is to find innovative processes to the energy storage. In this framework, materials with high dielectric permittivities are interesting for the development of devices such as hyper-capacitors. The project is devoted to the study of the dielectric response of some nanocomposites based on perovskites. In the context of a research in EDF R&D, the goal of this PhD position is to understand the microscopic and nanometric properties of these materials and connect them with microscopic high capacities.

The student will have to use first-principles modelling (Hartree-Fock, Density Functional Theory, ...) to understand the structural and electronic properties of the materials and their influence on the dielectric responses. The work will focus on three topics: a) study of various defects in different perovskites; b) study of the surfaces and interfaces properties of these materials and c) influence of the temperature, pressure, ... on the properties.

The work has both an applied and a theoretical aspect. This is why the PhD will be co-supervised by EDF R&D and the Université de Pau et des Pays de l'Adour (UPPA), represented by Philippe Baranek and Professor Michel Rérat, respectively. Most of the time the PhD will take place at the department of Materials and Mechanics of Components (MMC) of EDF R&D (in Moret – sur – Loing, near Fontainebleau, south of Paris, France) and supervised by Philippe Baranek but periods of work at the UPPA and in the Group of Theoretical Chemistry of Turin, supervised by Professors Michel Rérat and Roberto Dovesi have also to be envisaged for the programming part.

The expected starting date is the 1st October 2010

The candidate must have a background in nano-materials and nano-objects sciences, and a skill for programming. Knowledge of the first-principles methods and/or molecular modeling is recommended.

The interested candidate must send us a curriculum vitae with a cover letter and a list of two contacts for references.

Contacts :

Philippe Baranek, EDF R&D, Département MMC, Avenue des Renardières, 77818 Moret-sur-Loing Cedex, France.

Phone : 00 (33) 1 60 73 76 08

Email : philippe.baranek@edf.fr

Professor Michel Rérat, IPREM UMR5254, Université de Pau et des Pays de l'Adour, av. du Président P. Angot, 64053 Pau Cedex, France

Phone : 00 (33) 5 59 40 78 46

Email : michel.rerat@univ-pau.fr

Professor Roberto Dovesi, Dipartimento di Chimica IFM, Università di Torino and NIS, via P. Giuria 7, 10125 Torino, Italy

Phone: 00 (39) 011 670 7560

Email : roberto.dovesi@unito.it