

Density Functional Theory for Material Design in the Field of Applications for Energy

Research area

Ab initio simulations on massive parallel supercomputers, has become in the recent years, a powerful investigation tool widely used both for basic or applied research in the field of condensed matter.

The BigDFT package, developed in the framework of an European project coordinated by L_Sim, is at present in its production version and is routinely used in hybrid and parallel computers.

The Laboratory is at present involved in several projects (funded either by French or European Funding Agencies) related to the topic of electronic structure calculations for materials of interest in energy conversion. The recent oil crisis and the global necessity to find new green energy sources encourage the INAC institute to dedicate his research efforts in the direction of renewable energies. In the L_Sim lab, several efforts are ongoing to perform studies in this direction. BigDFT is a code with optimal features of reliability and precision, suitable to address different issues connected to material design for **photovoltaic** applications or **energy storage** applications.

For more details about ongoing work, visit http://inac.cea.fr/L_Sim/

Application conditions

For postdoctoral positions, the net salary range is 2,100€ - 2,400€ per month, depending on seniority, qualification and experience. Positions are available immediately but the starting date has to be scheduled with a minimum of three months in advance. The applicant must have strong skills in quantum physics, atomistic simulations and solid state physics, licensed by a PhD or an acknowledged research experience in the domain. A good knowledge of computer programming and environment is considered as an extra merit.

Interested candidates should send curriculum vitae, list of publications (preprints of unpublished papers are also accepted, but in a separate list) and arrange for two to three references addressed to:

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Clarification or further details can be obtained via email to pascal.pochet@cea.fr