Postdoc position in ab-initio simulation and code development

« Computation of Raman spectra on thin-layers and polycrystals »

Duration: 2 years (one-year contract renewable). Extension for a 3rd year under conditions.

Beginning of contract: From January 2023

Location: CEA DAM Île-de-France (Paris area, France)

Subject: Raman spectroscopy is an experimental measurement method based on the interaction of a laser with vibrational modes of a solid in order to obtain information about its crystal structure or chemical composition. At CEA Leti, Raman spectroscopy is an important step in the characterization of thin-layers developed for applications in microelectronics and microsystems, such as 2D layers, epitaxial layers or polycrystalline materials. Partnerships with industrialists are emerging so that Raman spectroscopy can be integrated into the monitoring of production processes.

The comparison of experimental spectra with theoretical predictions allows a much finer analysis, and the need for a spectra modeling tool is growing. The ABINIT software (www.abinit.org) has already been widely used to calculate Raman spectra from density functional theory (DFT).

ABINIT is an international collaborative project, in which CEA DAM is one of the main developer group. The project consists in providing CEA Leti with spectra calculated with ABINIT on materials of interest. For that purpose, it is necessary to deal with systems with many atoms (up to a few hundreds) in the crystal lattice in order to take into account the two-dimensional or disordered feature, which will require a first development in the code.

This postdoc objectives are:
- restructuring and then optimization of the code to deal with large systems
- automation of production processes and result analyses
- production of theoretical Raman spectra on materials of interest
- interaction with experimental team from CEA Leti

The applicant will work daily in Paris aera at the CEA DAM Île-de-France and will have to travel occasionally to the CEA Leti in Grenoble, France, to interact with experimentalists.

Expected profile: The applicant should have obtained a PhD in condensed matter physics for less than 3 years, with a strong component in ab-initio numerical simulation. Knowledge of standard Density Functional Theory methods is required, and development experience with Fortran or C/C++ is recommended. A strong interest in high performance computing is a plus.

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To apply or obtain additional information: Contact by email with CV and a research activity description. Offer Details:
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