Quantum simulation of resistive memories based on 2D materials

We are inviting applications for a **postdoc position** in a joint project at IMEP-LaHC and Leti-CEA in Grenoble. The successful candidate will perform DFT simulations of ***atomristors***, i.e., vertical memories based on 2D materials sandwiched between metal contacts. The applications of these devices range from low-energy and flexible non-volatile memories to radio-frequency switches for high frequency communications. The research, under the supervision of Alessandro Cresti and François Triozon, will focus on the role of disorder in determining the conduction properties of low-resistance and high-resistance states of these memories.

More specifically, the postdoc will perform ***ab initio*** and **quantum transport simulations** to study the effect of defects as vacancies or grain boundaries, in different 2D materials as transition metal dichalcogenides, between metallic vertical contacts. The *ab initio* simulations will be performed on Quantum ESPRESSO or ABINIT codes and SIESTA code. The quantum transport simulations, based on the Green's function approach, will be performed with TranSIESTA or in-house developed codes.

Different metals for the two contacts (as Au, Ni, Ti, Ag and Pt) and the use of 2D monolayers or multilayers (with both insulator and conductive geometrical phases) as well as heterostructures will be considered. In particular, the **following defects**, which can trigger the switching or, in case of conductive geometrical phases in the low resistance state, affect the conductance, will be investigated:

- **domains with geometric conductive phase** within the 2D material, with particular focus on their stability,
- **grain boundaries** due to the different orientation of the 2D material flakes, which, from experimental measurement, have typically a diameter of few tens of nanometers,
- **vacancies** in the 2D material, with possible migration and replacement with metal atoms from contacts.

The postdoc will flank the work of a third-year PhD student within the national project SWIT about *atomristors* for RF switches. She/he will also benefit from experimental results within the same project and other internal projects, and contribute to guide the design of performant devices.

Our ideal candidate:

- holds a PhD in condensed matter physics, electronic engineering or a related discipline,
- has strong experience with DFT simulations, in particular with SIESTA and preferably applied to 2D materials,
- has some programming experience with Fortran and Python,
- is very motivated and enjoys team work.

The position is for two years (one year plus one renewable year after evaluation). The starting date is flexible, with a first evaluation of the candidatures received by 01/04/2023. Evaluation of later candidatures is however possible if the position still available. We offer a competitive salary in a vibrant and stimulating work environment.

Interested candidates are welcome to submit their application, including a complete CV with list of publications, a cover letter stating their interest in the position, and at least one recommendation letter at the email addresses below indicated.

IMEP-LAHC

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