Postdoctoral opening in Computational Photovoltaics

A postdoctoral position in Computational Photovoltaics is available at Laboratoire d'Ondes et Matière d'Aquitaine (LOMA) at the University of Bordeaux, France. Funded by <u>Agence Nationale</u> <u>de la Recherche</u>, within the project "ORGAVOLT", the position is for 12 months (at a gross salary of about 2500€/month) and several possibilities for extending it can be envisaged. The starting date is January 2014, or as soon as possible afterwards.

We are looking for a highly motivated candidate, eager to interact with his/her future team mates, and with a drive to explore and contribute new methods and ideas. A background in computational materials science and scientific computing and coding is necessary. Further, some knowledge of many-body perturbation theory and Green function methods constitutes an advantage.

The project is a multi center collaborative effort between partners at Université de Grenoble (Grenoble, France), Universidad del País Vasco (San Sebastian, Spain) and Université de Bordeaux (Bordeaux, France). We investigate the first-principles prediction of the key properties of organic semiconductors that are used in bulk hetero junction solar cells, devices that <u>recently reached a</u> <u>12% efficiency</u>.

Bordeaux is a suitable environment for such challenging theoretical work because the synthesis of organic semiconductors is coordinated there, at the national level, by the group of <u>Georges Hadziioannou</u>. Besides, organic semiconductors constitute a key priority of the Bordeaux <u>Amadeus</u> initiative.

Your task will be the implementation of Hedin's GW approximation to predict the electronic band structure of organic semiconductors. This will be done using an unpublished extension to bulk of our algorithm that reduced the computational load from $O(N^4)$ to $O(N^3)$ scaling for molecules and clusters of *N* atoms (J. Chem. Phys. **135**, 74105, 2011). While the candidate will be based at LOMA, Bordeaux, the work will need close collaboration with, and frequent visits to, the <u>San</u> <u>Sebastian group</u>.

Applicants should send their CV, list of publications and two reference letters to Dietrich Foerster, <u>d.foerster@u-bordeaux1.fr</u>, LOMA, Université de Bordeaux I, Talence, Avenue de la Libération, France.

For further information on the "ORGAVOLT" project, please consult websites <u>at Bordeaux</u> and <u>Grenoble</u>. Interested candidates are encouraged to contact also the other team members for inquiries about the project:

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