PhD studentship on computational materials physics

CEA-Grenoble, FRANCE

A three year studentship is available towards the completion of a PhD degree in the area of theoretical and computational materials physics. The candidate will carry out a large-scale computational *ab initio* screening of defects in semiconductors, with the goal of inter-relating growth conditions, defect types and concentrations, and functional transport properties. This will lead to establishing a novel understanding of materials according to their prevalent defect types, and characteristic relationships between them and their functional properties. Innovative machine learning classification and regression algorithms will be used to unveil hidden trends and relationships and to accelerate the screening process. The project is expected to have a direct impact in the industrial development of new functional materials.

This position is based in Grenoble at N. Mingo's group, in close collaboration with the group of G. Madsen in Vienna. The research also involves close interaction with the Center for Materials Genomics at Duke University led by Prof. S. Curtarolo. Further information about the group's activities can be found on our website.

The city of Grenoble is located at the foot of the French Alps, being well connected to international destinations. Grenoble is an important European scientific center and it enjoys a rich cultural and natural environment.

Required qualifications:

MSc in physics, chemistry, materials science, or related discipline. An interest in theoretical modeling and programming. Proven programming experience is a plus.

To apply:

Send a full CV, a cover letter describing research interests and relevant experience, and the contact details for persons who could provide letters of recommendation, to natalio.mingo@cea.fr and ambroise.vanroekeghem@cea.fr . The call for applications is open until December 15th, 2017, and the position will be filled as soon as a suitable candidate is selected.