Post-doctoral position

Institute of Condensed Matter and Nanosciences

University of Louvain (Belgium)

Modeling novel van der Waals heterostructures

Research on graphene and other two-dimensional (2D) atomic crystals is intense and is likely to remain one of the leading topics in condensed matter physics and materials science for many years. Looking beyond this field, isolated atomic planes can also be reassembled into designer heterostructures made layer by layer in a precisely chosen sequence. A few heterostructures (often referred to as 'van der Waals') have recently been fabricated and investigated experimentally, revealing unusual properties and new phenomena. The goal of the present research project will be to investigate novel vdW compounds and to predict their promising physical properties.

The research will be carried out based on state-of-the-art first-principles calculations (and beyond) to investigate the novel structural, electronic, vibrational, magnetic and optical properties of vdW heterostructures. Using a multiscale approach, *ab initio* modeling will be used to enrich adjustable semi-empirical models in order to estimate the electronic transport in large-size vdW systems containing various sources of scattering (defects, stackings, spin-orbit coupling, electron-phonon coupling,…) as in real samples.

The work will be developed at IMCN (Institute of Condensed Matter and Nanosciences) in UCL (University of Louvain, Belgium) in the group of Prof. Jean-Christophe Charlier with strong interaction with the University of Liège (ULg, Prof. Matthieu Verstraete), and also within international collaborations with Prof. Stephan Roche (ICN2, Barcelona, Spain) and several experimental groups.

Profile: The candidate should be a theoretical physicist experienced in semi-empirical and/or DFT modeling (and beyond), preferably with good knowledge in quantum transport. No prior experience in modeling graphene or other 2D materials is required.

Starting date: the post-doc position will be open on October 1st 2015.
More information and application: jean-christophe.charlier@uclouvain.be