Secteur des Sciences
et Technologies

Invitation à la soutenance publique de thèse de

Monsieur Benoît VAN TROEYE

Master ingénieur civil physicien

Pour l'obtention du grade de Docteur en sciences de l'ingénieur et technologie

« First-principles investigation of interfaces in composite layered materials : application to lithium-ion batteries»

qui se déroulera

le jeudi 06 décembre 2018 à 15h

Auditoire SUD 09

Place Croix du Sud

1348 Louvain-la-Neuve

Membres du jury :

Prof. Xavier Gonze (UCLouvain), supervisor
Prof. Bernard Nysten (UCLouvain), chairperson
Prof. Jean-François Gohy (UCLouvain), secretary
Prof. Jean-Christophe Charlier (UCLouvain)
Prof. Matthieu Verstraete (Université de Liège, Belgium)
Prof. Nicholas Hine (University of Warwick, UK)

UCLouvain

Graphite is the prototypical anode material in lithium-ion batteries, as it can withstand hundreds of lithiation-delithiation cycles without breaking. Other materials, like silicon and black phosphorus (a layered material, like graphite), show much larger theoretical storage capacity than that of graphite. Still, this large specific capacity cannot be exploited in practice due to the important volume expansion associated with lithiation in these materials, leading quickly to their mechanical fracture. For sodiation, it has been recently demonstrated that a composite layered material constructed by stacking alternately graphene and phosphorene layers (the monolayers counterparts of graphene and black phosphorus) on top of the others combines both the advantages of graphite and black phosphorus (good cyclability and high capacity storage) [1]. Still, the origin of these improved performances was unknown at that time.

In this thesis, I investigate using first-principles computations (Density Functional Theory) the nanoscopic origin of these improved performances. It is found that the graphene layers do not only play the role of an electrical conductivity enhancer but also that of an elastic buffer in the composite layered material. In addition, an original intercalation process is identified at the interface between graphene and the lithiated phase of phosphorene. I predict that the material with the perfect alternation between graphene and phosphorene layers should show the most interesting properties for lithium-ion battery applications . In addition, an extension of the Frenkel Kontorova model is proposed to investigate the interface nature between graphene and phosphorene, as well as that between other 2D materials.