Secteur des Sciences et Technologies

Invitation à la soutenance publique de thèse de

Monsieur Viêt-Anh HA

Master of Science in Engineering Physics

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

« High throughput computing for high mobility p-type transparent conducting materials»

qui se déroulera
le mardi 07 mai 2019 à 15h30
Auditoire BARB 94
Place Sainte Barbe, 1
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Jury members :

Prof. Geoffroy Hautier (UCLouvain), supervisor
Prof. Gian-Marco Rignanese (UCLouvain), supervisor
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Prof. Xavier Gonze (UCLouvain), secretary
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In this thesis, we investigate transparent conducting materials (TCMs) which are the need of many modern technologies and devices. These are semiconductors which can combine both high visible transparency and electrical conductivity/mobility. While *n*-type TCMs (oxides) have been utilized in many applications such as solar-cells, touch screens *etc.*, their counterpart, *p*-type TCMs, is performing poorly in carrier mobility. This impedes the development of many modern technologies such as transparent solar cells. We, therefore, target on design of high mobility *p*-type TCMs. Using DFT in combination with other computational methods, we suggest new practical design principles for high mobility *p*-TCMs, particularly oxides. We hope that these principles can accelerate progress in this field, especially in the era of computational materials sciences nowadays. Moreover, we also extend our vision by exploring non-oxide zone instead of being bound to the traditional space of oxides. We set up high throughput computing framework based on DFT and beyond DFT methods such as hybrid functional, G0W0, electron-phonon interaction, semi-classical transport. Starting from a large database of (>34000) crystalline structures, we implement a series of computations for non-oxide compounds and sort out some materials showing positive potentiality (searching for "a needle in a haystack"). In final, several candidates including BP, CaTe and Li3Sb are identified as promising *p*-type TCMs. These binary compounds exhibit *p*-type dopability, low hole effective mass (high hole mobility) and high transparency in thin-film samples. Our results might inspire future works and convince people in community of TCMs that there are still plenty of rooms in non-oxide space.