



Secteur des Sciences
et Technologies

Invitation à la soutenance publique de thèse de
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Master : ingénieur civil physicien à finalité spécialisée

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

« FIRST-PRINCIPLES COMPUTATION OF THE ELECTRONIC
TRANSPORT IN
SEMICONDUCTORS FROM ELECTRON-PHONON COUPLING »

qui se déroulera
le jeudi 23 septembre 2021 à 15h30
Auditoire SUD 19
Place Croix du Sud
1348 Louvain-la-Neuve

Jury members :

Prof. Geoffroy Hautier (UCLouvain), supervisor
Prof. Gian-Marco Rignanese (UCLouvain), supervisor
Prof. Xavier Urbain (UCLouvain), chairperson
Prof. Xavier Gonze (UCLouvain), secretary
Prof. Matthieu Verstraete (ULiège, Belgium)
Prof. Feliciano Giustino (University of Texas, USA)
Prof. Clément Lauzin (UCLouvain)



First-principles computations have emerged as a formidable tool for characterizing known and new materials and hence accelerating materials discovery. The electronic transport is among the most important properties for many technological applications. Therefore, a correct ab initio description of the transport properties of functional materials is crucial. In this work, we develop a new methodology to compute the intrinsic carrier mobility in semiconductors. The intrinsic transport is limited by the scattering by phonons and requires precise knowledge of the electron-phonon (e-ph) coupling in the material.

In semiconductors and insulators, the e-ph coupling is largely influenced by long-range interactions that have to be taken into account for accurate physical results. We go beyond the state-of-the-art dipolar Fröhlich interactions and include the treatment of quadrupolar fields in the first-principles e-ph coupling matrix elements in semiconductors. We apply our formalism to Si (nonpolar), GaAs, and GaP (polar) and demonstrate that electron mobilities show large errors if dynamical quadrupoles are not properly treated.

We also inspect the particular case where the e-ph coupling is so strong that the carriers self-localize and form small polarons. In the framework of transparent conducting oxides (TCOs), we demonstrate using well-known physical models that, in certain circumstances, materials exhibiting transport by small polarons offer a better combination of transparency and conductivity than materials conducting through band transport. We link this surprising finding to the fundamentally different physics of optical absorption for band carriers and small polarons. Our work rationalizes the good performances of recently emerging small-polaron Cr-based p-type TCOs and outlines design principles for the development of high-performance TCOs based on transport by small polarons. This opens new avenues for the discovery of high-performance TCOs especially p-type.