

# Invitation à la soutenance publique de thèse

Pour l'obtention du grade de Docteur en Sciences de l'Ingénieur

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Erasmus Mundus Master of Science in Nanoscience and Nanotechnology

## Ab Initio study of structural, thermodynamical, vibrational and electronic properties of CZTS

Photovoltaics, which convert sunlight into electricity, is one of the sustainable solutions to meet the global energy demand. In this framework,  $\text{Cu}_2\text{ZnSnS}_4$  (CZTS) has attracted considerable attention as a potential earth-abundant and non-toxic absorber material for thin film solar cells due to its favorable electronic and optical properties. Despite the considerable efforts, its efficiency has remained low. One possible explanation is the cation disorder in the system. In this thesis, we investigate this issue using two different approaches.

Firstly, since the arrangement of cations over several possible sites makes first-principles density functional theory (DFT) calculations impractical, we rely on a combination of DFT with cluster expansion and Monte Carlo methods to evaluate the thermodynamical properties. We identify the phase transitions and also analyze the nature of bandgap change with temperature.

Secondly, since Raman and infrared spectroscopies are considered to be robust techniques for analyzing disorder in CZTS, we compute the vibrational properties of well-known ordered structures of CZTS (kesterite, stannite and PMCA) and compare them with experiments. The effect of different exchange-correlation functionals is also addressed both in a qualitative and quantitative manner. Further, newer features arising from the spectra of many other structures show a better matching with experiments.

Both approaches highlight the importance of cation disorder on the properties of CZTS.

**Jeudi 28 septembre 2017 à  
15h00**

Salle de séminaire ISV (B.059)  
Bâtiment Carnoy  
Croix du Sud, 5  
1348 Louvain-la-Neuve



### Membres du jury :

Prof. Gian-Marco Rignanese (UCL), promoteur  
Prof. Bernard Piraux (UCL), président  
Prof. Geoffroy Hautier (UCL), secrétaire  
Prof. Xavier Gonze (UCL)  
Prof. Jean-Christophe Charlier (UCL)  
Prof. Michel Houssa (KUL, Belgique)  
Prof. Susanne Siebentritt (University of Luxembourg, Luxembourg)