



Secteur des Sciences  
et Technologies

Invitation à la soutenance publique de thèse de

**Monsieur Nicolas DARDENNE**

Master complémentaire en nanotechnologie

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

« Electronic and optical properties of organic materials from first-  
principles for green energy »

qui se déroulera

**le vendredi 15 mars 2019 à 15h**

**Auditoire SUD 08**

**Place Croix du Sud**

**1348 Louvain-la-Neuve**

Membres du jury :

Prof. Gian-Marco Rignanese (UCLouvain), supervisor

Prof. Jean-Christophe Charlier (UCLouvain), supervisor

Prof. Bernard Nysten (UCLouvain), chairperson

Prof. Geoffroy Hautier (UCLouvain), secretary

Prof. Jean-François Gohy (UCLouvain)

Prof. Xavier Blase (Institut NEEL – CNRS Grenoble, France)

Prof. David Beljonne (UMons, Belgique)

The need for better green energy technologies has become critical for the future of our society. One of the most promising renewable energy sources is the unlimited sunlight. Combined with the concept of clean technologies, organic photovoltaics naturally emerge as one of the potential green energy sources. Green batteries made with clean and abundant materials could also be developed in order to store the current generated by the solar cells in a more sustainable way. In this work, two quantum *ab initio* methods are presented and used in order to speed up the accurate characterization of organic molecules. On the one hand, the  $\Delta$ SCF method, based on the density functional theory (DFT), allows for the computation of the ionization energy and the electronic affinity of localized systems such as organic molecules. On the other hand, for other excited state properties, it is necessary to go beyond DFT using many-body perturbation theory within the *GW/BSE* approximations to obtain precise values.

New organic batteries built with radical polymers display voltage around 3.6 V while showing high charging and discharging rate performance and long life-cycle. In this work, the  $\Delta$ SCF technique is used to estimate the open cell voltage of various nitroxide radical polymers used as cathode materials. The computed voltages are predicted in good agreement with the experimental values. With the intent to improve the performance of these batteries, molecular engineering is then performed for building newly designed organic radicals and their properties are investigated. As for the organic solar cell, a better understanding of the effects that impact the behavior of excitonic states is needed to improve our comprehension of the working principles of a donor-acceptor blend. The splitting of excitons into free charges is supposed to be mediated by the available CT states created by the energy level offsets between the active materials. In this work, it is demonstrated that accurate optical gaps of organic solids can be computed with the *GW/BSE* method. Finally, organic interfaces made of various donors and acceptors are studied. In particular, it is shown that the *GW/BSE* is able to predict the lowest CT state energy which is directly related to the open cell voltage of the solar cell.