UNIVERSITÉ DE NAMUR

PhD student position within the Laboratory for Computational Modeling of Functional Materials at the Namur Institute of Structured Matter of the University of Namur

Profile

We are looking for a skillful and highly motivated PhD student who has some expertise in computational chemistry/physics.
The candidate is expected to:

- have an expertise in either [or both] electronic structure calculations (Time-Dependent Density Functional Theory, wavefunction-based methods…) or [and] molecular dynamics simulations.
- be autonomous.
- be a dynamic and enthusiastic team player.
- be highly motivated by conducting a collaborative research project with experimentalists.
- have good communications skills in English (reading, writing and speaking).
- to be able to present clearly his research results.
- be familiar with Linux operating system.
- to have an experience with programming languages (C, Fortran, Python, Perl, bash,…).

Conditions of eligibility

Latest starting date: 01/10/2024
Contract : two-year fixed-term contract, renewable
Category : PhD student. **CANDIDATES MUST NOT HAVE A PHD.**
Net Salary per month: 2417.07€ (PhD grant)
Hiring conditions: The candidate will be supervised by Prof. Olivier and will be hired first for a period of two years. If you are not European, you will need a unique permit to work at University of Namur. The single permit application procedure can take up to 4 months from the moment the application file is complete.

The research project that the candidate is going to pursue will take place within a “Action de Recherche Concertée (ARC)”* project together with Prof. Ludovic Troian-Gauthier and Prof. Benjamin Elias from the Université Catholique de Louvain. The project itself will deal with the investigation of materials for photo-triggered processes such as clean fuels production, phototherapy, decontamination, and photocatalysis using a joint experimental-computational approach. To do, we will model every elementary electron transfer process

taking place in the excited state of these molecules and leading to the formation of radical cation and anion species able to participate in chemical reactions, considering a combination of quantum chemical methods and molecular mechanics/dynamics methods.
*Funder : Fédération Wallonie Bruxelles

References

[1] Morton, C. M.; Zhu, Q.; Ripberger, H.; Troian-Gautier, L.; Toa, Z. S. D.; Knowles, R. R.; Alexanian, E. J.; J. Am. Chem. Soc. **2019**, 141, 13253-13260
[2] Troian-Gautier, L.; Swords, W. B.; Meyer, G. J.; Acc. Chem. Res. **2019**, 52, 170-179.
[3] Aydogan, A.; Bangle, R. E.; Cadranel, A.; Turlington, M. D.; Conroy, D. T.; Cauët, E.; Singleton, M. L.; Meyer, G. J.; Sampaio, R. N.; Elias, B.; Troian-Gautier, L.; J. Am. Chem. Soc. 2021, 143, 15661-15673.
[4] Olivier, Y.; Yurash, B.; Muccioli, L.; D'Avino, G.; Mikhnenko, O.; Sancho-García, J. C.; Adachi, C.; Nguyen, T. Q.; Beljonne, D.; Physical Review Materials **2017**, 1, 075602.
[5] Di Meo, F.; Fabre, G.; Berka, K.; Ossman, T.; Chantemargue, B.; Paloncýová, M.; Marquet, P.; Otyepka, M.; Trouillas, P. ; Pharmacological Research **2016**, 111, 471-486.
[6] Di Meo, F. ; Lemaur, V. ; Cornil, J. ; Lazzaroni, R. ; Duroux, J.-L. ; Olivier, Y. ; Trouillas, P. ; J. Phys. Chem. A **2013**, 117, 2082.

Laboratory for Computational Modeling of Functional Materials

Prof. Yoann is heading the Laboratory for Computational Modeling of Functional Materials (LCMFM) at the University of Namur since the 1st of July 2019. The LCMFM is part of the Namur Institute for Structured Matter (NISM). The research activities within the LCMFM are focused on the theoretical description of the structural and opto-electronic properties of π-conjugated organic materials in the bulk, at organic/organic interfaces as well as charged and optical excitation dynamics and transport properties. The group develops and applies multiscale computational techniques to investigate these topics, combining first principle electronic structure calculations ((Time-Dependent) Density Functional Theory, wavefunction-based methods,…), molecular dynamics simulations, Kinetic Monte Carlo techniques as well as tight-binding electronic structure calculations beyond the single molecule scale parameterized from first principle calculations.
The research within the LCMFM benefits from the full access to the computing facilities from the "Consortium des Équipements de Calcul Intensif" (CÉCI), a consortium of high-performance computing centers of the Universities from the French Community of Belgium supported by the F.R.S-FNRS and the Walloon Region and the Tier-1 CENAERO supercomputer of the Fédération Wallonie-Bruxelles which are entirely used for theoretical calculations in Chemistry and Physics.

Application

The candidates are requested to send by e-mail to yoann.olivier@unamur.be and before the 10th of September 2024 latest: an updated CV including publications track record together with a motivation letter and two reference letters from professors or previous supervisors.

The selection procedure is as follows: 1. Analysis of applications based on, 2. Auditions of selected candidates, 3. If needed: testing.

Complementary information

Prof. Yoann Olivier – Tel: +32(0)81/72 45 34
Email: yoann.olivier@unamur.be