UNIVERSITÉ DE NAMUR

Postdoctoral position within the Laboratory for Computational Modeling of Functional Materials at the Chemistry and Physics departments of the University of Namur.

Profile

We are looking for a skillful and highly motivated postdoctoral researcher who obtained a PhD 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.
- 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: 01/06/2021
Contract : For one year, maximum 2 years
Category : Postdoctoral researcher. **CANDIDATES MUST HAVE ALREADY A PHD.**
Net Salary per month: ~2700 €
Hiring conditions: The candidate must be experiencing an international scientific mobility meaning he/she shall not have resided or carried out his/her main activity (job, studies…) in Belgium for more than 24 months during the last 3 years directly before the first stay as a Postdoctoral fellow. The first hiring period shall start at the latest exactly 6 years after obtaining the academic degree of doctor, after the defense of a thesis. The maximum period of time mentioned above is extended for one additional year per childbirth and/or adoption. The candidate will benefit from a postdoctoral grant from the hosting university. This grant will be exempted from taxes but subject to the employee social security.

Research project

The research project that the candidate is going to pursue will deal with the investigation of new emitters exhibiting thermally activated delayed fluorescence (TADF) for organic light-emitting diodes applications. In particular, we will be interested in the interplay between the chemical structures of the emitters and the host materials, the electronic properties as well as the mechanistic aspects leading to the upconversion of otherwise lost to heat, triplet excited states into emissive singlet excited states.

References

[1] Olivier, Y.; Sancho Garcia, J.C.; Muccioli, L.; D'Avino, G.; Beljonne, D. J. Phys. Chem. Lett. 2018, 9, 6149.
[2] Olivier, Y.; Yurash, B.; Muccioli, L.; D'Avino, G.; Mikhnenko, O.; Sancho-Garcia, J.C.; Adachi, C.; Nguyen, T.Q.; Beljonne, D. Phys. Rev. Mater. 2017, 1, 075602.
[3] Evans, E.W.; Olivier, Y.; Puttisong, Y.; Myers, W.K.; Hele, T.J.H.; Menke, S.M.; Thomas, T.H.; Credgington, D.; Beljonne, D.; Friend, R.H.; Greenham, N.C. J. Phys. Chem. Lett. 2018, 9, 4053.
[4] Pershin, A.; Hall, D.; Lemaur, V.; Sancho-Garcia, J.C.; Muccioli, L.; Zysman-Colman, E.; Beljonne, D.; Olivier, Y. Nat. Commun. 2019, 10, 597.
[5] B. Yurash, H. Nakanotani, Y. Olivier, D. Beljonne, C. Adachi, and T.Q. Nguyen. Adv. Mater. 2019, 31, 1804490.
[6] S.M. Suresh, D. Hall, D. Beljonne, Y. Olivier, and E. Zysman-Colman. Adv. Funct. Mater. 30 (2020) 1908677.

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 both the Chemistry and the Physics departments of the University of Namur as well as 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 before the 1st of April 2019 latest: an updated CV including publications track record together with a motivation letter and two reference letters from professors or previous supervisors.

Complementary information

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