PhD student position within the Laboratory for Computational Modeling of Functional Materials at the Namur Institute of Structured Matter of the University of Namur and Laboratory for Chemistry of Novel Materials at the University of Mons.

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: 01/07/2024
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 both Prof. Olivier and Prof. Beljonne and formally will be hired first for four years at the University of Namur but will share equally his time between the University of Namur and the University of Mons.
If you are not European, you will need a unique permit to work at University of Namur and the University of Mons. The single permit application procedure can take up to 4 months from the moment the application file is complete.

Research project

The research project that the candidate is going to pursue will take place within a "Projet de Recherche (PDR)"* from the FRS-FNRS. This is a collaborative project together with two experimental groups based in the United Kingdom, namely, the group of Profs. Friend, Rao and Bronstein from the University of Cambridge and the group of Dr. Emrys Evans at the University of Swansea. The project itself will deal with the characterization of radical molecules exhibiting a high emission quantum yield for applications in organic light-emitting diodes (OLEDs) devices and/or quantum information sciences (QIS). The project will rely on the findings made in a recently published article [1]. Essentially, we will seek for materials sustaining (i) positive (ferromagnetic) exchange interactions between spin centers in order to stabilize and to manipulate- high-spin excited states at room temperature; (ii) low-lying electronic excitations with prominent radiative decay rates and small non-radiative decay rates for efficient light emission; and (iii) resonant energy level alignment between the radical emissive electronic states and the chromophore high-spin excited states for efficient interstate conversion using a combination of computational methods. We will establish a feedback loop with the experimental partners at the University of Cambridge and University of Swansea to fine tune the design strategies of such optically active compounds.
*Funder : Fédération Wallonie Bruxelles

References

[1] S. Gorgon, K. Lv, J. Grüne, B.H. Drummond, W.K. Myers, G. Londi, G. Ricci, D. Valverde, C. Tonnelé, P. Murto, A.S. Romanov, D. Casanova, V. Dyakonov, A. Sperlich, D. Beljonne, Y. Olivier, F. Li, R.H. Friend, E.W. Evans, Nature (2023) accepted.
[2] X. Ai, E. W. Evans, S. Dong, A. J. Gillett, H. Guo, Y. Chen, T.J.H. Hele, R.H. Friend, F. Li, Nature 563, 536 (2018).
[3] A.J. Gillett, A. Pershin, R. Pandya, S. Feldmann, A.J. Sneyd, A.M. Alvertis, E.W. Evans, T.H. Thomas, L.S. Cui, B.H. Drummond, G.D. Scholes, Y. Olivier, A. Rao, R. Friend, and D. Beljonne, Nat. Mater. 21 (2022) 1150.
[4] M. Franz, F. Neese and S. Richert, Chem. Sci. 13, 12358 (2022).
[5] M.R. Wasielewski, M.D.E. Forbes, N.L. Frank, K. Kowalski, G.D. Scholes, J. Yuen-Zhou, M.A. Baldo, D.E. Freedman, R.H. Goldsmith, T. Goodson III, M.L. Kirk, J.K. McCusker, J.P. Ogilvie, D.A. Shultz, S. Stoll and K. B. Whaley, Nat. Rev. Chem. 4, 90 (2020).

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.

Laboratory for Chemistry of Novel Materials

The activities within the Laboratory for Chemistry of Novel Materials (LCMN) are focused on the theoretical description of the structural and opto-electronic properties of π-conjugated organic materials in the bulk, organic/organic and organic/substrate interfacial properties as well as graphene electronic and transport properties. 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. Experimental researches are also pursued to understand and control the morphology of thin films based on π-conjugated organic materials for device preparation (OLEDs and solar cells) at the Materia Nova research center. During the last ten years, LCMN participated to more than fifteen European projects in the domain of organic electronics (FP7 SINGLE, FP7 ONE-P, FP7 ORION, FP7-MMM@HPC, FP7-Genius, FP7 SUPERIOR, FP7-UPGRADE) and was coordinator of the project FP7 MINOTOR. LCMN was also among the team laureate for the Descartes prize of the European commission in 2003 which rewards the excellence in the collaboration between university and industry.

Application

The candidates are requested to send by e-mail to yoann.olivier@unamur.be and david.beljonne@umons.ac.be before the 15th of May 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
Prof. David Beljonne – Tel: +32(0)65/ 37 38 72
Email: david.beljonne@umons.ac.be