

« Quantum chemical investigation of the second-order nonlinear optical & chiroptical properties of helical organic molecules »

A two-year post-doctoral position is available at the University of Namur in the newlyestablished Namur Institute of Structured Matter (<u>http://nism.unamur.be</u>) and particularly the Theoretical Chemistry Lab (<u>http://www.unamur.be/en/sci/chemistry/lct</u>).

Details of the project. In the frame of a multidisciplinary framework involving the University of Bordeaux, the project aims at developing original nanometer-sized aromatic helical architectures featuring unique second-order nonlinear optical & chiroptical properties that will be studied via cutting-edge spectroscopic techniques that are hyper-Rayleigh scattering in solution and second-harmonic generation of chiral surfaces, in order to build switchable chiroptical functional surfaces and perform NLO-resolved chiral molecular dynamics studies at interfaces. The present position concerns the quantum chemistry aspects, *i.e.* using and developing quantum chemistry methods to predict and analyze the second-order nonlinear optical & chiroptical properties of oligomeric helices.

Offer. The grant will be about 2500 € per month. The candidate must be in an "international scientific mobility situation" hence being able to benefit from the postdoctoral grant [should not have resided or carried out his/her main activity (job, studies...) in Belgium for more than 24 months during the 3 last years]. Moreover, the beginning of the hiring period should, at the latest, be exactly 6 years after obtaining the academic degree of doctor, after defense of a PhD thesis. The candidate will be working in the research group of Prof. Benoît CHAMPAGNE and use computational facilities provided by the HPC consortium of the Fédération Wallonie-Bruxelles, including those of the Scientific Computing Platform of our University.

Requirements. Highly motivated candidates with i) a PhD in Theoretical/Quantum Chemistry or in related areas, ii) an expertise in response properties (ideally electric, magnetic, and mixed responses) modelling methods, iii) an expertise in multi-scale simulation methods is an asset, iv) abilities to communicate (sufficient level in English combined with good pedagogical skills) and to work in a team, including theoreticians and experimentalists, while v) an expertise in scientific programming (fortran, C++, python, ...) in view of writing new codes and of modifying existing ones is an asset.

How to apply. Interested candidates should send their curriculum vitae, list of publications, cover letter explaining why you feel being the right person for this position, and a list of, at least 2, contact references e-mails (in a single PDF file) to Prof. Benoît CHAMPAGNE, <u>benoit.champagne@unamur.be</u>. Candidates are advised to apply as early as possible. The selection process will start immediately.