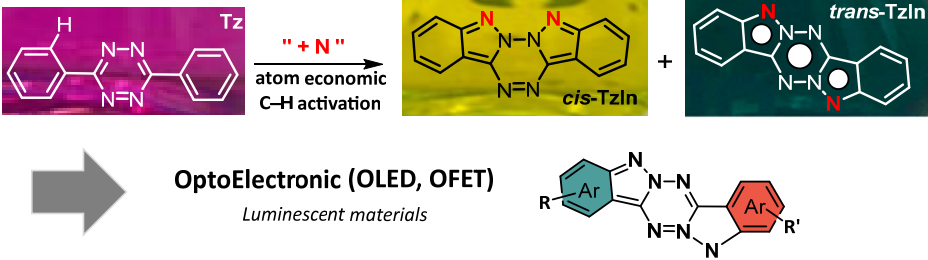


Recrutement prévu dans le cadre du projet recherche :
Synthesis and Electronic Properties of Novel Aza-Aromatics
ANR PI AZA

Job title	Post-doc in Theoretical studies of innovative s-tetrazine derivatives.
Ref	offreEmploi_2023.07_postdoc_ANR PI AZA
Job type (PhD, Post-doc, Engineer)	Post-doc
Contract duration (months)	12 months
Qualifications (Master degree, PhD...)	PhD
Salary	Gross monthly salary 2 600 €
Job hours (full time/ part time)	Full time
Employer	UBFC – Université Bourgogne Franche-Comté
Host Laboratory	Institut de Chimie Moléculaire de l'Université de Bourgogne (ICMUB)
URL Host Laboratory	http://www.icmub.com/en/team/ocs-organometallics-catalysis-stereochemistry.html
Address Host Laboratory	Institut de Chimie Moléculaire - UMR CNRS 6302 9 avenue Alain Savary – BP 47870 – 21078 DIJON CEDEX
Job description	<p>Theoretical studies of innovative N-rich derivatives for optoelectronic</p> <p>A postdoctoral position in Computational Chemistry is available in the group of Pr. Paul Fleurat-Lessard (http://pfleurat.free.fr/index.php) in Dijon at the Institut de Chimie Moléculaire de l'Université de Bourgogne (http://www.icmub.com/en/) (France).</p> <p>The successful candidate will apply electronic structure theory, post-HF and (TD)-DFT methods to investigate organometallic chemistry mechanism and photophysical properties of tetrazine derivatives in the context of the Pi-Aza project.</p> <p>This project aims at designing new Pi-conjugated heterocycles (Scheme 1) from greener processes (C–H activation) to generate materials which are potentially applicable energy materials and optoelectronics (photovoltaic applications, OLED and OFET).</p> <p>The program is based on the rational development of molecules with high N-content based on the s-tetrazine core (Tz) such as tetrazo[1,2-b]indazoles (TzIn).^[1]</p> <p>This new class of compounds can be obtained by regioselective functionalization in <i>ortho</i>-position of the aryl moieties by relevant transition metals, reagent or functionalization.^[2,3] We will adopt a bottom-up approach</p>

	<p>in which the rational choice of the substituents will be driven by quantum computations. The theoretical analyses of the electronic structure of the molecules (AIM, ELF and NCI approaches) and their excited states (TD-DFT, SOS-CISD, ADC,...) will be used to predict the photophysical and packing properties.</p> <p style="text-align: center;">Sustainable synthesis of new N-rich TetrazolIndazole</p> <div style="text-align: center;">  <p style="text-align: center;"><i>Scheme 1 – Sustainable synthesis of N-rich tetrazo[1,2-b]indazoles for optoelectronics applications</i></p> </div> <p>Bibliography</p> <p>[1] A. Daher, A. Bousfiha, I. Tolbatov, C. D. Mboyi, H. Cattey, T. Roisnel, P. Fleurat-Lessard, M. Hissler, J.-C. Hierso, P.-A. Bouit, J. Roger <i>Angew. Chem. Int. Ed.</i> 2023, <i>62</i>, e202300571. [2] a) J. Roger et al., <i>Angew. Chem. Int. Ed.</i> 2016, <i>55</i>, 5555; b) J. Roger et al., <i>ACS Catal.</i>, 2017, 7, 8493; [3] C. D. Mboyi, D. Vivier, A. Daher, P. Fleurat-Lessard, H. Cattey, C. H. Devillers, C. Bernhard, F. Denat, J. Roger, J.-C. Hierso <i>Angew. Chem. Int. Ed.</i> 2020, <i>59</i>, 1149–1154.</p>
<p>Qualifications</p>	<ul style="list-style-type: none"> - PhD in theoretical or computational chemistry or physics - some knowledge of organometallic chemistry - Be a curious and self-driven person - Experience in modeling of photophysical properties - Some programming skills would be a plus.
<p>Supervisor(s)</p>	<p>Pr Paul FLEURAT-LESSARD – Mail : Paul.Fleurat-Lessard@u-bourgogne.fr</p>
<p>Candidate profile</p>	<p>The candidate should hold a PhD in theoretical chemistry and/or physical-chemistry. He/She must have some knowledge in organometallic chemistry. He/she must be interested in the theoretical investigation of reaction mechanisms, as well as photophysical properties. Experience in programming will be appreciated. A good level in English and/or French is necessary.</p>
<p>Keywords</p>	<p>DFT, reaction mechanism, Photophysical properties, N-rich heterocycles</p>
<p>Application deadline</p>	<p>August 15th 2023</p>
<p>Starting job</p>	<p>October 1st 2023</p>

Application
*Depending on the
type of position*

Post-doctoral Position

Please send the following documents (all in one PDF file) by e-mail to:
Paul.Fleurat-Lessard@u-bourgogne.fr

- 1) For EU candidates: Copy of your national ID card or of your passport page where your photo is printed.
For non-EU candidates: Copy of your passport page where your photo is printed.
- 2) Curriculum Vitae.
- 3) Letter of motivation relatively to the position.
- 4) Copy of your PhD degree if already available.
- 5) 2 recommendation letters from previous scientific supervisors.

If you have questions regarding the application, please contact the supervisor(s).