



Postdoc position in computational quantum chemistry in Rennes

Funding:	ANR-DFG (Agence Nationale de la Recherche, France - German Research Foundation) 1 year full-time position - expected starting date: end of 2021
Location:	Inorganic theoretical chemistry team (CTI) Institute of Chemical Sciences of Rennes (ISCR) https://iscr.univ-rennes1.fr/inorganic-theoretical-chemistry-cti
Supervisor:	Karine COSTUAS , CNRS senior researcher https://orcid.org/0000-0003-0338-0494

Subject: The project entitled “Coordinated luminescent supramolecular assemblies based on pre-organized Cu(I) precursors stabilized by ligands of main group elements” is a multidisciplinary project gathering synthetic chemists, photophysicists and computational chemists. The hired post-doctoral fellow will be fully associated in the project which aims at designing new flexible polymetallic supramolecular assemblies based on luminescent Cu (I) precursors combining luminescence and detection properties. He/she will be in charge of the study of the structure-properties relationships (photo-physical properties) of synthesized or targeted systems at the ground state and excited states by computational chemistry tools, mainly DFT. This work implies a close connection with the experimental partners of the project. This computational work will provide a better understanding of the mechanisms that leads to luminescence and of the other properties notably magnetic properties. An in-silico computational work will be also performed to guide the molecular design. The hired researcher will be in charge of the supervision of students involved in the project.

Publications of the consortium linked to this project:

- *Solid State Highly Emissive Cu(I) Metallacycle: Promotion of Cuprophilic Interactions at the Excited States*; M. El Sayed Moussa, S. Evariste, H.-L. Wong, L. Le Bras, C. Roiland, L. Le Polles, B. Le Guennic, K. Costuas, V. W.-W. Yam, C. Lescop, *Chem. Commun.*, **2016**, DOI: 10.1039/C6CC06613E
- *Adaptive coordination-driven supramolecular syntheses toward new polymetallic Cu(I) luminescent assemblies*; S. Evariste, A. Khalil, M. Elsayed Moussa, A. Chan, E. Hong, H.-L. Wong, B. Le Guennic, G. Calvez, K. Costuas, V. W.-W. Yam, C. Lescop, *J. Am. Chem. Soc.*, **2018**, DOI: 10.1021/jacs.8b06901
- *Intramolecular rearrangements guided by adaptive coordination-driven reactions toward highly luminescent polynuclear Cu(I) assemblies*; M. El Sayed Moussa, A. Moustafa Khalil, S. Evariste, H.-L. Wong, V. Delmas, B. Le Guennic, G. Calvez, K. Costuas, V. W.-W. Yam, C. Lescop, *Inorg. Chem. Front.*, **2020**, DOI: 10.1039/c9qi01595g
- *Luminescent vapochromic single crystal to single crystal transition in one-dimensional coordination polymer featuring the first Cu(I) dimer bridged by an aqua ligand*; S. Evariste, A. M. Khalil, S. Kerneis, C. Xu, G. Calvez, K. Costuas, C. Lescop, *Inorg. Chem. Front.*, **2020**, DOI: 10.1039/d0qi00691b
- *Coordination-Driven Supramolecular Syntheses of New Homo- and Hetero- polymetallic Cu(I) Assemblies: Solid-State and Solution Characterization*; A. M. Khalil, C. Xu, V. Delmas, G. Calvez, K. Costuas, M. Haouas, C. Lescop *Inorg. Chem. Front.*, **2021**, DOI: 10.1039/D1QI00937K



Work environment: This post-doctoral work is funded by an international ANR-DFG project and will take place within the framework of a collaboration involving other research teams in Rennes and Regensburg in Germany. The candidate will be hosted at Institute of Chemical Sciences de Rennes on the Campus Beaulieu at the University of Rennes 1 (<https://iscr.univ-rennes1.fr/>).

All resources (hardware, software packages) needed to complete the work are available at the CTI team. The team gathers fifteen staff members, and twelve PhD students / post-docs working in quantum computational chemistry and material science (from molecules and hybrids to solid state compounds). The Institute of Chemical Sciences of Rennes is a multidisciplinary laboratory that gathers more than 215 academic researchers and more than 600 members that makes it one of the largest laboratories in France dedicated to chemistry.

Qualifications: Admission requires a PhD in molecular physics/chemistry or physical/theoretical chemistry. Applicants should be highly motivated and have experience in computational chemistry. Previous experience in TD-DFT simulations and/or rationalization of luminescence will be an advantage. Good communication skills are required for this collaborative project, in particular written and spoken English.

Contact information: Interested candidates should contact Karine Costuas (karine.costuas@univ-rennes1.fr) and apply at <https://bit.ly/3ALinHo> as soon as possible