M2 and PhD Fellowship in Computational Chemistry at the University of Grenoble

Title : Theoretical studies of Copper Centers

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Institut : Department of molecular chemistry (https://dcm.univ-grenoble-alpes.fr)
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Objectives :

Copper centers are commonly found in enzymes and inspire new biomimetic catalysts. Theoretical studies of these systems are essential to support experimental data, get mechanistic insight. However due to the switch between singlet and triplet states as for example for dicopper oxygen complexes, calculations are not trivial. One solution is to use a broken-symmetry approach. The aim of this thesis is to propose the implementation of protocols combining this approach of broken symmetry with new innovative theoretical methods, such as the use of localized orbitals and the metadynamics to determine the mechanism involved.

The studied systems are part of a collaboration with the group of C. Belle (https://dcm.univ-grenoble-alpes.fr/research/cire-team/research-areas/reactivite-et-mecanismes-complexes-bio-inspires). On one hand, we are interested in understanding the reactivity of novel copper-based catalysts capable of effectively oxidizing strong C-H bonds under mild and eco-compatible conditions. On the other hand we want to study one of the key steps of the biosynthesis of melanins by tyrosinase, a binuclear copper enzyme.

The candidate will interact regularly with the experimental team, will learn a large panel of computational methods, DFT, QM/MM , MD simulations and will manipulate several computing codes (for instance: Gaussian, CP2K, Amber).

Further information and application:

Contact Helene Jamet by email (Helene.jamet@univ-grenoble-alpes.fr) ASAP. Please attach a letter of motivation, CV.