Open PhD position – University of Nantes (France)

Subject: **Design of a third generation of a new class of negative photochromes**
Position: PhD position in computational chemistry – 36 months starting in September 2019.
Location: Laboratory: CEISAM, UMR CNRS 6230 University of Nantes (France),
http://www.sciences.univ-nantes.fr/CEISAM/, ModES Team.
Contact: Adèle Laurent, Adele.Laurent@univ-nantes.fr

We are looking for highly motivated candidates for a PhD position funded by the French national agency (ANR). The project focuses on the understanding with mutli-scale methods of the dynamics behavior of a protein that is only fluorescent in presence of a specific ligand.

Research context and program

The project concerns a ligand-induced fluorescent protein (LIFP) that has been recently discovered. The LIFP protein emits intense and bright green light once a ligand is bound to the protein. The ligand is an indirect marker of various human liver functions and has an antioxidant role. The new LIFP is therefore a promising direct medical tool to track liver disease as well as a probe to detect cardiovascular diseases. The PhD candidate will model this new LIFP class for the very first time, to understand its electronic, spectral, and conformational properties, as well as to design new ligands or mutants able to enlarge the panel of possible applications.

The goals will be fulfil thanks to the state-of-the-art multi-scale computational tools including: i) robust and/or refined quantum mechanics methods to model the ligand antioxidant and excited-states properties; ii) hybrid QM/MM schemes to account for surroundings; iii) molecular dynamics to assess the impact of conformational changes; iv) free energy calculations to estimate the energy barrier while ligand entering in the protein; and v) docking to explore new ligands, and so explore new applications. More precisely within the QM/MM methods, a method taking into account explicitly for electronic polarization of the surrounding of the ligand will be employed.

Applicant

The applicant should have **a master in physics, computational/theoretical chemistry, or bioinformatics**. Proven experience in molecular modeling are a prerequisite, as well as in scientific computing and programming (C++,Python, perl). The candidate should have a strong interest in the simulation of optical properties of dyes in condensed phase (solvent, protein). She/he should be highly motivated and show initiative. Good oral and written communication skills are necessary. Applications should be addressed to adele.laurent@univ-nantes.fr. Interested candidates should send their CV, a cover letter describing their research interests and motivation, and the names of two reference persons to the contact e-mail address.
