RESEARCH LABORATORIES

Laboratory For Computational Molecular Design

Prof. Clemence Corminboeuf

http://isic.epfl.ch/lcmd

clemence.corminboeuf@epfl.ch

General areas: Theoretical and Computational Chemistry

Research themes

Our research interests focus on the developments and applications of accurate and innovative chemical theories and methods for rationally designing molecule with predefined macroscopic properties. Our challenges are 1) Overcoming the deficiencies of Kohn-Sham Density Functional Theory; 2) Devising methods and schemes to tune molecular properties in order to enable 3) Applications to the design of novel functional material.

As for the elaboration of novel materials, we focus primarily on pi-electron systems that account for numerous unique properties as exemplified by organic semiconductors, photovoltaic devices, and gas storage materials. In this context, the development of quantum chemical methods enabling the direct probing and tuning of electron delocalization effects on the properties of materials/(bio)molecules represent an exceptional prospect.

Methodology of work/special instrumentation

LCMD welcomes motivated master students, who will enjoy working in a Linux/Unix computer-oriented scientific environment for using and/or developing computational chemistry software in the Fortran programming language.

Recent examples of MSc/PhD thesis