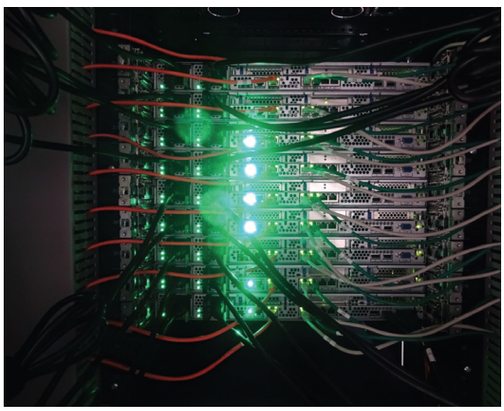
Laboratory of Theoretical Chemistry – Unit of Theoretical and Structural Physical-Chemistry – Namur Institute of Structured Matter – UNamur

Chemistry supporting simulation and new materials

With about ten researchers, twenty international publications a year and as many presentations at international congresses, the Laboratory of Theoretical Chemistry (LCT) of UNamur is currently leading about ten research projects.

Focused on multidisciplinary research and training for research, the LCT is developing theoretical research methods to implement them in simulation codes/programmes, to understand the properties of matter, to deduce property-structure relationships and to design new materials with target properties.

For this purpose, the main lines of research are molecules/materials for nonlinear optics, vibrational spectroscopy, electronics and molecular photonics. Within the context of an ARC inter-university collaboration with the teams of Prof. J. Wouters (UNamur) and T. Leyssens (UCLouvain), LCT researchers are studying the phenomena of solid state photochromism and thermochromism in order to optimise these. They are also developing quantum chemistry methods to calculate the responses of molecules, surfaces and solids to magnetic fields and geometric deformations. This enables the simulation of high-level optical responses and vibrational signatures of chiral structures. Moreover, they are studying molecular switches which have the potential to be active elements in sensors and in logical devices (on a molecular level).



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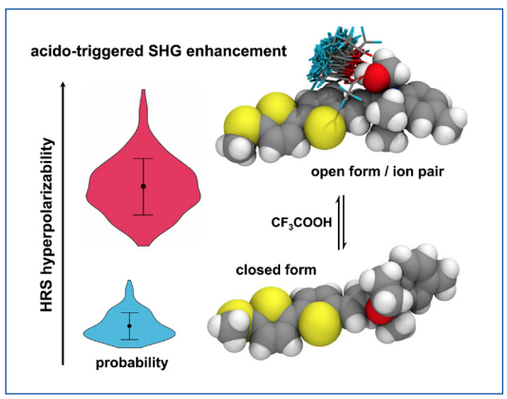
Hercules, HPC server of the PTCI (technology platform for High-Performance Computing) of UNamur, is an integral part of the CECI (Consortium of Equipment and High-Performance Computing) of the Walloon-Brussels Federation.



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Molecular switch showing a nonlinear optical contrast response

The LCT has numerous research international partners: Bordeaux and Angers (France), Osaka (Japan), Krakow (Poland), Sherbrooke (Canada), Sfax and Tunis (Tunisia), Bologna (Italy), Calcutta (India), etc. At national level, its participation in three successive projects in the context of the Belspo Interuniversity Attraction Poles, has led to supervising a thesis under joint supervision with UHasselt. The subject is TADF (Thermally Activated Delayed Fluorescence) and it aims at enhancing the efficiency of organic light emitting diodes. The LCT is also involved with a team from KULeuven working on fluorescent proteins, used for medical imagery.

The collaboration with Osaka University has proved to be particularly productive. First, it enabled the researchers to forecast in theory that compounds with intermediate diradical character should present high third-order nonlinear optical responses – which was confirmed by experiments some years later. From then on, it became possible to apply a magnetic field to modify the electronic and optical properties of these materials that are still not well known, even if the aspects of stability and implementation of these new phenomena still need to be fine-tuned.

Then, with the University of Bordeaux, a collaboration revealed methods of triggering molecular switches and generating high second-order nonlinear optical contrasts. In addition to the transformations brought about by the variation in pH or irradiation, the researchers have shown the capacity of intelligent molecules to recognise and distinguish cations (a prediction that is awaiting experimental confirmation). On the other hand, the demonstration that chiral vibrational spectroscopies can provide information on polymer chain structures has been confirmed by experiments.

At the moment the LCT is facing two challenges: first, that of taking into account several levels, both of size and time, in simulations and second the development of simulation codes that could be used reliably by non-specialists. This is the reason for the series of software programmes DrawMol, DrawSpectrum, etc. developed by Dr V. Liégeois (FNRS researcher) and available on Mac. Using this powerful graphic interface, you can visualise and construct molecular structures. This is a boon for extending scientific research to ordinary citizens!

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