

### **Static and dynamical properties of molecular systems through different levels of representation**

I will present three research themes investigated through collaborative and independent research works. The talk will cover (a) multiresolution analyses of electron density distributions, (b) molecular docking and Molecular Dynamics simulations of host-guest systems, and (c) Kinetic Monte Carlo simulation of the synthesis of two-dimensional graphitic sheets.

a. Changing the resolution or smoothing degree of an electron density distribution (EDD) can reduce the number of parameters needed in molecular similarity analyses, e.g., through reduced molecular graph representations. I will also present a recent work on the topology of EDDs, analyzed at different thermal displacement factors and crystallographic resolutions, showing how the properties of non-covalent interactions are affected by these modifications.

b. Molecular docking and Molecular Dynamics simulations are common methods used to model dynamical properties of proteins and host-guest systems. Collaborative works about the identification of inhibitors of a protein-protein system, as well as simulations of guests embedded in organic cages will be presented.

c. Finally, a collaborative study using Kinetic Monte Carlo simulations will be presented. This work is based on preliminary quantum mechanical calculations of the kinetic parameters that describe the synthesis of graphitic carbon nitride sheets.

### **Curriculum vitae of Prof. Dr. Laurence Leherte**

After the defense of my PhD thesis on Molecular Dynamics of zeolitic systems (Laboratory of Theoretical Chemistry, Dir. Prof. Jean-Marie André) in 1990, I spent two years as a postdoctoral researcher at the laboratory of Computational Imagery at Queen's University (Kingston, Canada) and the Cambridge Crystallographic Data Centre (England). I returned to the University of Namur to work in the laboratory of Computational Physical Chemistry (Dir. Prof. D. Vercauteren) where I developed research on the topological analysis of electron density distributions at various levels of resolution, with applications to molecular similarity and complementarity, as well as to Molecular Dynamics of protein systems. In 2018, I moved to the laboratory of Structural Biological Chemistry (Dir. Prof. Johan Wouters) where I now work on the application of electron density analysis tools to the study of molecular interactions, as well as on Molecular Dynamics simulations of proteins and supramolecular systems. I am currently appointed as university lecturer at the University of Namur.

