Dr Gilles FRAPPER

Applied Quantum Chemistry group, IC2MP – Poitiers U., CNRS

https://orcid.org/0000-0001-5177-6691

gilles.frapper@univ-poitiers.fr

BIOGRAPHY

Gilles Frapper was born in Saint-Cado, south Bretagne. He studied chemistry at Rennes U. (PhD in Applied Quantum Chemistry 1996. Pr. Jean-Yves Saillard and Dr. Jean-François Halet). Since 1997, he is at Poitiers University, having previously held research positions at NRC Ottawa (Dr. John Tse group) and Georgetown U. in Washington D.C. (Pr. Miklos Kertesz). He taught introductory chemistry, and he (still) enjoys teaching theoretical chemistry and material sciences. His primary research focus is to comprehend the atomic arrangements in molecular and solid-state compounds in conjunction with their properties. He specializes in the field of Computational Materials Discovery, predicting bidimensional systems and bulk materials under pressure. Nowadays, he combines evolutionary (genetic) algorithms, random generators, machine-learning interatomic potentials and quantum mechanics calculations to design new materials with specific properties and applications.

When Darwin meets Mendeleev: predicting materials from evolutionary algorithms and first-principles calculations. *Illustrations*: Pb-N and Li-C-N systems under pressure (45 min. in French, but slides in English).

By Dr Gilles FRAPPER

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Using numerical simulation to determine the crystal structure of a compound, based on the sole knowledge of its chemical composition, is a major challenge in materials science. The task is far from trivial: it involves identifying the lowest-energy structural arrangement from among millions of possible structures. To illustrate this challenge, the arrangement of twenty atoms in a box - a repeating lattice of variable shape and volume - can a priori generate more than 10^{21} possible structures that lie on the potential energy surface (PES). If it took 1 hour of computing time to numerically determine the energy associated with each optimized structure, the computing time required would exceed the age of the universe... The problem is therefore: how to access the lowest energy well (global minimum on the PES) while monopolizing a minimum of computational resources?

This talk will discuss a self-learning method for exploring the PES of a crystalline compound, an evolutionary (genetic) algorithm combined with DFT calculations. I will briefly outline the conceptual basis of this CSP algorithm, which is based on the concepts of the Darwinian evolutionary theory. I will then illustrate its use by presenting some recent results from work carried out in my *Applied Quantum Chemistry* group: the exploration of the Lead-Nitrogen binary phase diagram under pressure (0-100 GPa), the emergence of novel compositions in the Li-C-N ternary system at 50 and 100 GPa, the ABH_3 hydrides “perovskites” under pressure, with/without perovskite’structure…, and the recovery of selected phases to ambient conditions; the bonding and electronic properties of the *in silico* compounds using basic and state-of-the-art theoretical chemistry tools (Lewis, VSEPR, ELF, COHP, COBI, …), and so on...