Machine Learning Approaches for Nanoparticle Modelling

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The use of Artificial Intelligence (AI) in scientific research has advanced considerably in recent years, across disciplines ranging from the exact sciences to the humanities and medical sciences. *Machine Learning* (ML), a subfield of AI, encompasses a set of computational algorithms designed to develop models capable of efficiently learning from data or past situations. ML-based approaches have proven particularly valuable in materials science, where they support theoretical predictions and/or data exploration for the design and characterization of new materials.

Within the *Surface, Interface and Nano-object* group at CEMES in Toulouse, our research focuses on the growth and investigation of the structural, physical, and chemical properties of surfaces and interfaces, nano-objects, and their interactions with atoms or molecules (adsorption, self-organization, growth, and functionalization). To address these topics, we combine experimental and theoretical approaches over a broad range of systems, from spintronic to biomedical applications.

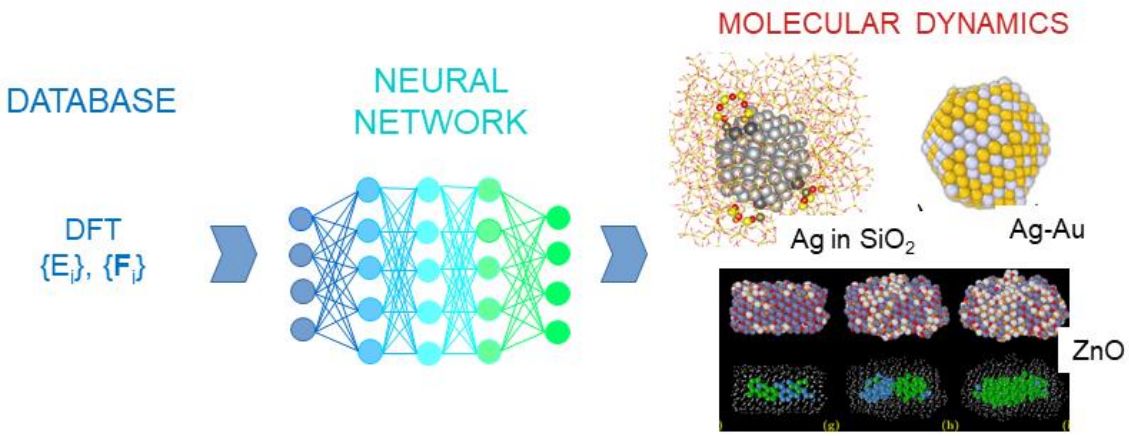

Fig.1. Schematic illustration of the development of neural-network interatomic potentials for the nanoparticles modelling.

In this presentation, after a brief introduction to the fundamentals of ML, I will present recent research examples conducted within our group [1–6], where we implemented ML methods to assist in the modelling of nanoparticles. In particular, by using ML-based interatomic potentials, we can now access larger spatial and temporal scales, thereby facilitating direct comparison between simulated models and experimental results.

References

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