Accelerating the Structure Exploration of Diverse Bi–Pt Nanoclusters via Physics-Informed Machine Learning Potential and Particle Swarm Optimization

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Bimetallic nanoparticles (NPs) have received tremendous interest in the fields of catalysis, energy materials and biomedical applications, thanks to their synergistic interactions between their constituents. Our interest lies particularly in the Bi-Pt system, shown, for exemple, to have enhanced catalytic activity over the simple Pt catalyst in the electrooxydation of formic acid[1], have been employed to monitor temperatures in reactor melt wires and have been synthesied as radio-enhancers for radiotherapy[2].

Theoretical investigations of this system are rare and difficult to realize. The potential energy landscape of such a system is vast and complex, notably due to the mixing of two elements with differing crystal structures (rhombohedral bismuth and cubic face centered platinum) and the abundance of structural variety emerging from it (Core-shells, Janus and other alloy configurations). Thus, we employ machine learned interatomic potentials (Ml-IPs), trained on DFT level data to maintain accuracy, while significantly improving calculations costs. In our work, we focused on the the Chebyshev Interaction Model for Efficient Simulation (ChIMES)[3], a physically informed ML potential based on multibody interaction cluster expansion and Chebyshev polynomials. We successfully trained the model on the data scarce system, iteratively improving and growing our training data via active learning. Once capable of delivering accurate predictions of energies and forces, we paired the ChIMES model with a global optimisation algorithm, CALYPSO[4] leveraging its exploratory capabilities for an efficient simulation of the system's structural space.

Finally, we exploited all the data accumulated on the system, including spectral properties (IR, DOS and VDOS), structural and shape descriptors (e.g coordination numbers, radial distances...) and electronic properties (e.g cohesion energy, band gap...) to obtain a machine-led classification of the structural types observed. This data led approach, via principal component analysis and k-mean clustering, is compared with a manual classification of the structures obtained into Core-shells, Janus and mixed alloys. These results and methods are further explained in an upcoming article[5]. We now aim to further understand the impact of data selection on our model training, compare its behavior and suitability with foundational models pretrained on large databases and to advance the study of the system, notably by including NPs with varying metallic ratios, sizes and potentially the chemical environment.

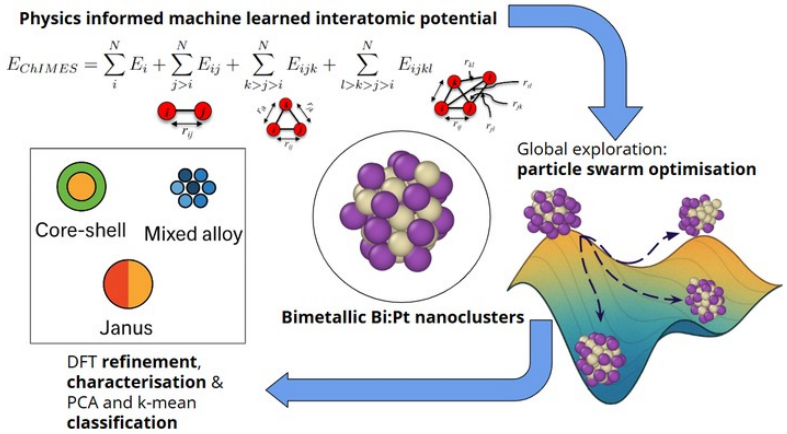

Figure 1: Graphical abstract of the methods used

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