Comparison of two machine learning interatomic potentials for bimetallic nanoparticles

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Heavy metal nanoparticles (NP) see a lot of developments and interests as radiosensitizers for radiotherapy. A new bimetallic Bi:Pt NP coated with PEG-based ligands was developed at ISMO, Paris Saclay using radiolysis. But what effects does the synthesis method have on the organization and surface of the NP?

Theoretical studies of bimetallic nanoparticles have been lagging those seen for noble metal nanoparticles such as gold and silver nanoparticles. This is due to the complexity of multicomponent systems which make proper characterization far more difficult than homogeneous systems.

Machine learning interatomic potentials (ML-IAPs) are quickly gaining importance in the field of theoretical chemistry and material sciences, as they offer cheaper alternatives to commonly used DFT calculations. In addition, they are positioned to bridge the lack of adequate force fields for molecular dynamics of complex systems.

Using our DFT reference data (PBE/LANL2DZ/HayWadt-ECP) for 59 atom bismuth-platinum nanoparticles, we will compare the results from a non linear fitting process, using the multi layer neural networks of DeepMD[1], and the linearly fitted parameters of the Chebyshev interaction model for efficient simulation (ChIMES)[2;3].

We aim to provide a better picture on the suitability of the ML-IAPs available for bimetallic systems, weighing on the pros and cons of two design philosophies. In addition, we also intend to scale up our structural and vibrational results from the initial scope of DFT models to the experimental conditions of our systems counting tens or hundreds of thousands of atoms, far beyond the current capabilities of DFT methods.

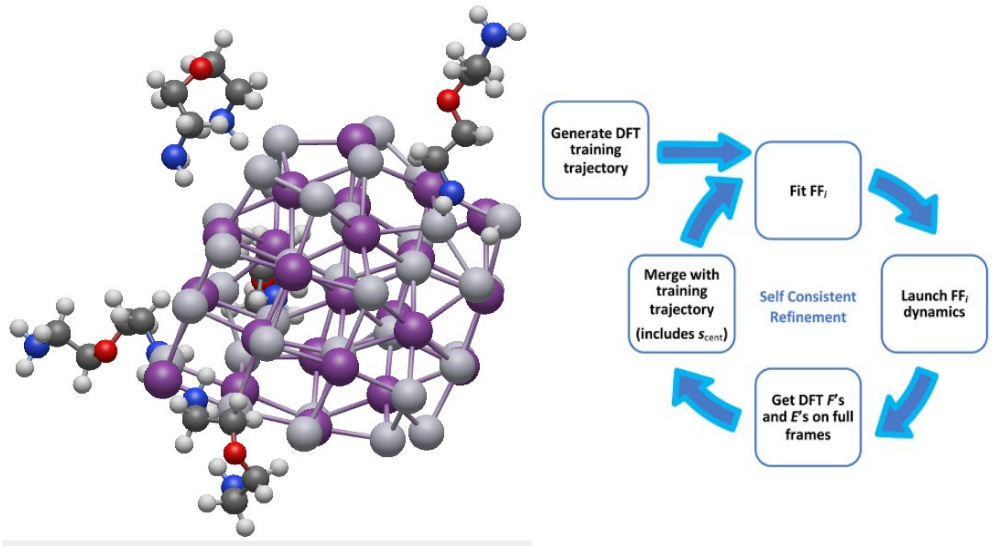

Figure: Model of the optimized bimetallic NP and scheme of the ChIMES refinement process

Keywords: Machine learned inter-atomic potentials (ML-IAPs); Heavy metal nanoparticles

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