Machine Learning Interatomic Potentials for Metal Nanoparticles

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Gold nanoparticles are of great interest in advanced radiotherapy where these nanoparticles are often used to enhance radiosensitivity. It has been demonstrated by experiments in our lab that interfacial water plays a central role in the production of OH radicals when irradiating solvated gold nanoparticles. Our group has experience simulating these systems using classical potentials [1,2,3]. However, these methods do not predict well the interaction energy between gold nanoparticles and water molecules. Due to the size of the systems and the timescale, direct first principle molecular dynamics simulations of these systems are prohibitively expensive; hence we employ in this work different machine learning strategies to tackle the problem:

- the delta-machine learning within the framework of Density Functional based Tight Binding (DFTB) model
- the Chebyshev Interaction Model for Efficient Simulation (ChIMES), a physics-informed machine learning interatomic potential (ML-IAP) [4,5]
- and the deep neural network ML-IAP of DeepMD model [6]

The main advantage of these machine learning potentials is that their cost is that of classical potentials, but their accuracy is comparable to quantum level calculations. In this work, we will present the characterization of the interaction energy and structural, dynamical and vibrational properties of the water surrounded gold nanoparticle using these machine learning methods [7]. A perspective of using these machine learning methods for studying the structure of bismuth-platinum nanoparticles is also presented [8].

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