Machine learning for protected metal nanoclusters: structure, dynamics, chemistry

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Ligand-protected noble metal nanoclusters, commonly termed as "monolayer-protected metal clusters" (MPCs), comprise a common set of structures exhibiting a metal core stabilized by an organic layer of ligand molecules. The choice of the metals defines the clusters' physical properties, such as the electronic, optical, and magnetic properties, whereas the organic ligand shell defines their solubility and functionality with the surrounding environment. MPCs currently provoke widespread fundamental interest as tunable nanomaterials because they can be engineered, in principle, with atomic precision. Here, I will discuss our recent efforts to model gold-based MPCs with machine learning methods based on both experimental and DFT data. I start from a rule-based heuristic method to predict a correct atomistic structure of the metal-ligand interface, validated with experimental datasets (1), continue on description of atom dynamics via accelerated machine learning potentials and force fields trained from DFT data (2,3), and finish by using graph theory to predict hydrogen adsorption, relevant for understanding the first steps of electrochemical hydrogen evolution on gold-based MPC catalysts (unpublished work).

(1) S. Malola, P. Nieminen, A. Pihlajamäki, J. Hämäläinen, T. Kärkkäinen, H. Häkkinen, "A method for structure prediction of metal-ligand interfaces of hybrid nanoparticles", Nature Comm. 10, 3973 (2019).

(2) A. Pihlajamäki, J. Hämäläinen, J. Linja, P. Nieminen, S. Malola, T. Kärkkäinen and H. Häkkinen, "Monte Carlo Simulations of $Au_{38}(SR)_{24}$ Nanocluster Using Distance-Based Machine Learning Methods", J. Phys. Chem A 124, 4827-4836 (2020).

(3) A. Pihlajamäki, S. Malola, T. Kärkkäinen and H. Häkkinen, "Orientation Adaptive Minimal Learning Machine: Application to Thiolate-Protected Gold Nanoclusters and Gold-Thiolate Rings " https://arxiv.org/abs/2203.09788