Active Learning of Physics Aware Potentials for Nanostructured Systems: Application in Gas Sensing

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Key Words: ***Force Field, Molecular Dynamics, atomic clusters, gas/solid interfaces..***

Abstract

Sensing gas pollutants at the nanoscale is inherently a non-trivial task. Molecular Dynamics (MD) simulations might give critical insights and facilitate the design of such nanosensing devices. However, the accuracy of the MD simulation depends on the underlying force field (FF); the potential energy term describing the atomistic interactions. To address this, a generic active learning (AL) framework is proposed for developing force fields (FFs) for complex nanostructured molecular systems involving atomic-sized clusters and various gaseous molecules that constitute air pollutants, crucial for advancements in environmental technologies. The AL algorithm systematically trains and refined physics aware FFs on ***ab-initio*** Density Functional Theory (DFT) data, sampled via stochastic methods and using the FF itself. At each AL iteration, new candidate structures are generated via stochastic methods such as Monte Carlo or stochastic MD (Langevin dynamics). From these candidates, a small subset of them is selected for DFT labeling, performance evaluation and augmenting the dataset in the next iteration. The AL framework is applicable to various cases, producing FFs that can describe interactions of multiple character, within the atomic silver nanoclusters and cluster/gas hybrids, including cohesive, strong physisorption, and chemisorption interactions. [1] The considered classical models utilize a combination of physical descriptors and flexible potential terms, maintaining efficiency, accuracy and transferability. Their prediction accuracy is comparable to those of the ***ab-initio*** calculations and of advanced machine learning models, however, they preserve the computational efficiency of simple semi-empirical potentials. [2]

References

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