Chemically accurate simulations by machine learning correlated approximations

Dario Rocca

Ab initio molecular dynamics (AIMD) is vital for understanding a wide variety of physical systems, including sorption behavior in porous materials like zeolites and metal-organic frame works. Unfortunately, the low-cost density functional approximations that make it numerically feasible can also lead to quantitative and sometimes qualitative errors in calculations.
Here we introduce a method based on thermodynamic perturbation theory and machine learning that allows for the evaluation of finite temperature properties using high-accuracy/high-cost correlated wave-function methods. The power of this approach is illustrated on the case of the adsorption of small molecules in zeolites at room temperature, where we show that the random phase approximation (RPA) achieves a high level of accuracy by predicting values in excellent agreement with experiment.