

Optimization of VASPsol Solvation Free Energy Predictions

Eric Fonseca, Sean Florez, and Richard Hennig

Department of Material Sciences, University of Florida, Gainesville, FL

Density functional theory is a powerful tool for predicting material properties and reaction barriers, but it is often limited to small systems due to high computational costs. To address this issue, computational chemists often use continuum models to approximate the effect of solvent molecules on atomic systems. VASPsol is a polarizable continuum model that can be used within the plane-wave DFT code VASP. This work aimed to optimize the VASPsol cavity parameters by minimizing the error between predicted and experimentally measured solvation energies. We used the Truhlar Minnesota dataset and COSMO-SAC sigma-profile descriptors to featurize our molecular dataset. Recent work has shown that the sigma profile makes an excellent molecular descriptor for solvent-solute interactions. By analyzing the errors across different chemical groups, we can optimize VASPsol parameters for multiple solvents. Following this optimization, we can use our featurized dataset to examine the performance of our continuum model across various chemical moieties.