Physical Chemistry Seminar

Accurate predictions of QM/MM energies using a modified long-range ANI/MM neural network potential

Shahed Haghiri

Graduate Student, The Slipchenko Group

Purdue University

ANI is one of the promising machine-learned Neural Network Potentials (NNPs) that replace computationally expensive ab initio calculations by learning the complex correlations between atomic coordinates and electronic structure properties1. Such NNPs calculate the final energy as a sum of local environmental energies of each atom, leading them to be widely transferable to almost any molecule but at the cost of losing long-range interactions like electrostatic effects. This is due to the usage of Behler-Parinello symmetry functions to vectorize the molecules, which have a cutoff that ignores all interactions further than 5.2 Angstroms. In our previous work, we designed an ANI-1x-based network that could predict the Coulomb and polarization components of the solute-solvent interaction energies and trained it on a set of small, solvated molecules2. This new ANI/MM network takes electrostatic potentials on each atom computed with the Effective Fragment Potential as an additional input feature. We extend the previous work to show how to utilize the ANI/MM developed network for predicting protein-ligand interaction energies. Here, we trained it on QM/MM energies for two protein-ligand systems, 2VTL/LZ5 and 4EK5/03K. The ANI/MM network predicts both energies and forces with singular kcal/mol accuracy.

References:

1.Gao, X.; Ramezanghorbani, F.; Isayev, O.; Smith, J. S.; Roitberg, A. E. TorchANI: A Free and Open Source PyTorch-Based Deep Learning Implementation of the ANI Neural Network Potentials. *J. Chem. Inf. Model.* **2020**, 60 (7), 3408–3415. https://doi.org/10.1021/acs.jcim.0c00451.

2.Haghiri, S.; Viquez Rojas, C.; Bhat, S.; Isayev, O.; Slipchenko, L., ANI/EFP: Modeling Long-Range Interactions in ANI Neural Network with Effective Fragment Potentials, J. *Chem. Theory Comp.* **2024**. DOI: 10.1021/acs.jctc.4c01052.

Wednesday, February 26, 2025 **10:30am** **BRWN 4102**

PURDUE UNIVERSITY | James Tarpo Jr. and Margaret Tarpo Department of Chemistry