Evaluation of Thermochemical Machine Learning Methods

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Motivation

For reliable applications of ML, methods need to properly predict conformational changes from non-equilibrium bond stretching to torsional barriers.

Molecules

- 17 bond stretches and 5 dihedral scans
- Test set consisted of benzene, methanol, methane, CO, H_2, ethylene, water, acetylene, hydrogen cyanide, N_2, ammonia, biphenyl, aspartame, sucrose, dialanine, and diglycine.

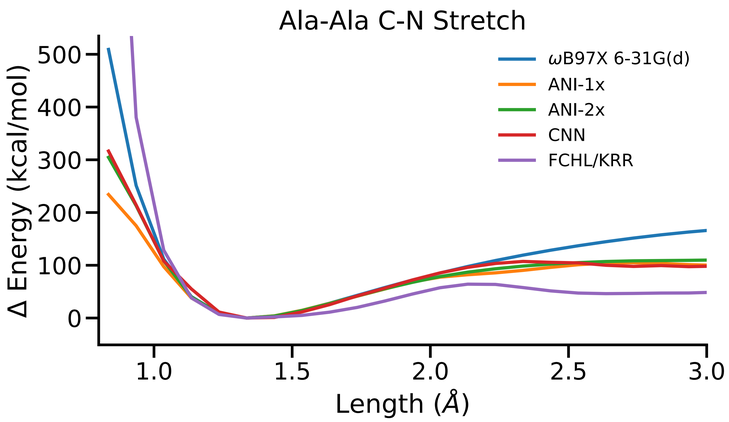
Bond Stretching

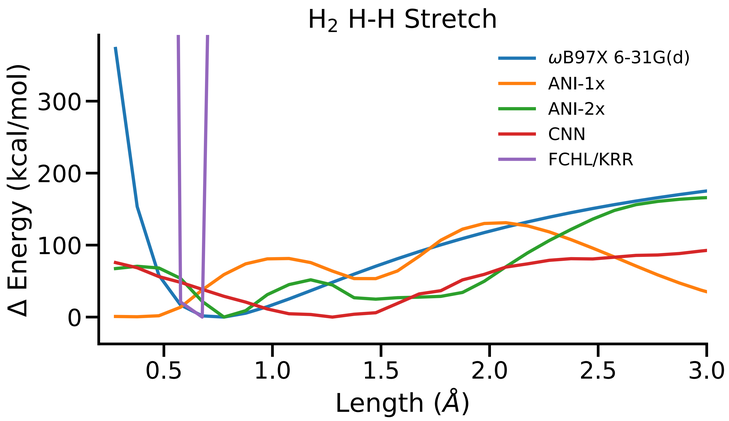
Methods	Median MAPE	r_0	Repulsive Wall	Attractive Forces
ωB97X 6-31G(d)	0.000	17	17	17
ANI-2x	0.002	17	13	17
BOB/BRR	0.227	0	5	5
FCHL/KRR	0.255	10	16	15
CNN	0.256	16	17	17
ANI-1x	0.265	16	11	17
BOB/KRR	0.313	1	9	11
BOB/RFR	43.88	2	3	0
BAND-NN	99.31	11	9	5
MMFF94*	100.0	14	17	0
GAFF*	100.1	13	17	0
ECFP/RFR	193.4	0	0	0

*Force Field methods for comparison

Methods ANI-1x, ANI-2x, FCHL, and CNN best demonstrated the ability to accurately predict energies while also predicting the repulsive and attractive forces of the potential energy curves.

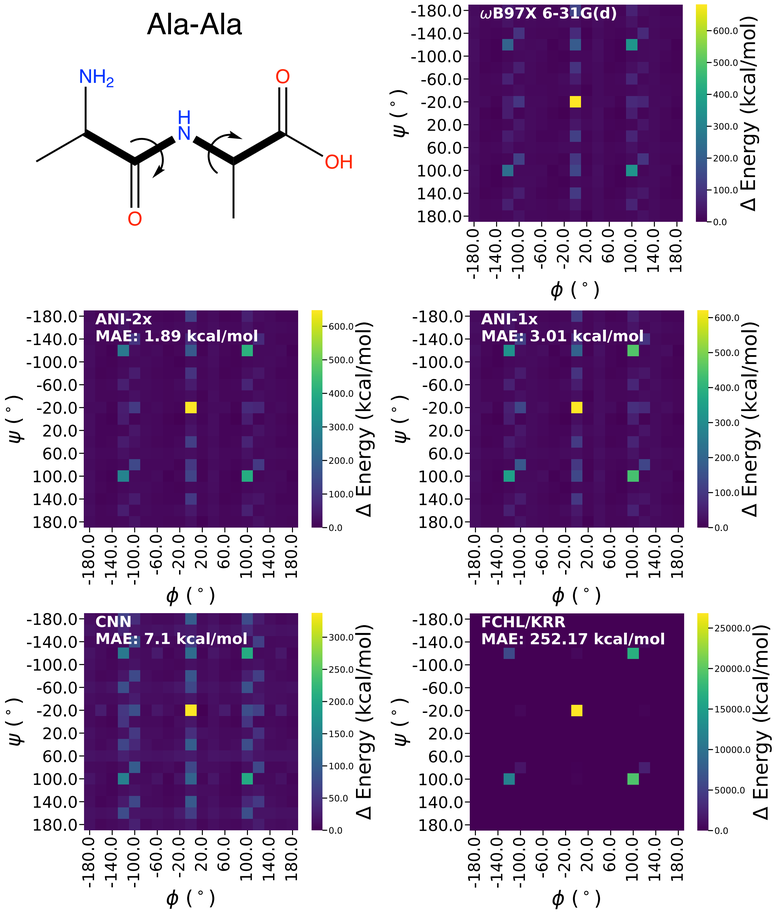
Potential Energy Curves





ML performance demonstrates the learning of chemical physics around r_0 and anharmonic bond stretching. While these methods performed adequately around r_0, there are issues predicting the extremes of bond stretching as well as motifs outside of the training set as seen with H_2. These issues should be addressed in the future through the inclusion of additional bonding motifs and long-range attractive forces in the training set.

2D Torsion Scans



The additional torsion sampling in the training of ANI-2x helped the model outperform the ANI-1x counterpart. Additional torsion sampling for methods CNN and FCHL should also provide a decrease in MAE allowing for these methods to gain additional quantitatively accurate.

Conclusion

ML performs well around the equilibrium bond length but struggles to predict long-range attractive forces and motifs outside of the training set.

Thanks

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