INTERNATIONAL INSTITUTE OF INFORMATION TECHNOLOGY
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R&D SHOWCASE 2021
Technology, Social Impact

Neural Network Potentials with DFT Accuracy at FF computational cost.

ABSTRACTS

In recent years, Deep learning (DL) has lead to a paradigm shift in many areas of science and technology, especially image, text, and speech recognition. Machine learning (ML), in general and Deep learning in particular are becoming increasingly popular in computational chemistry. These methods are ideal for representing quantum-mechanical (QM) interactions which enables us to model non-linear potential energy surface (PES).

OBJECTIVE

- ★ To estimate the accuracy of the NN potential compared to DFT reference calculations.
- ★ To highlight the true transferability of these models, all molecules considered in the test cases contain greater than eight heavy atoms.

MODEL

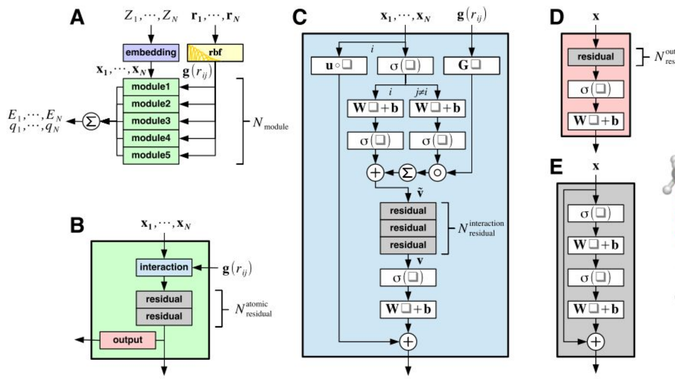

Fig 1:- A: Overview over the PhysNet architecture. B: Structure of a modular building block. C: Interaction block. D: Output block. E: Preactivation residual block (J. Chem. Theory Comput. 2019, 15, 3678−3693).

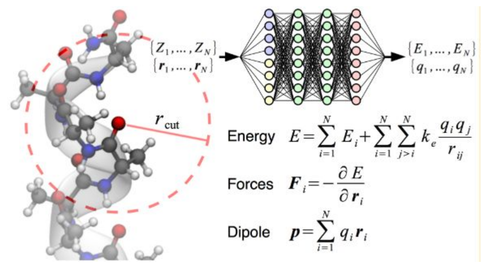

Fig 2:- Schematic representation showing energy prediction of the single atom under consideration using DL (J. Chem. Theory Comput. 2019, 15, 3678−3693).

RESULT

- ★ Subset of ANI-1 dataset containing DFT energies of ~20 million conformations. Each molecule has up to 8 heavy atoms containing H,C,N and O. Conformers up to 30 kcal/mol higher in energy from ground state are used (~7.6M points).
- ★ Accurate prediction of atomization energy with mean absolute error (MAE) of 0.43 kcal/mol on test set.
- ★ Random molecules with 10 heavy atoms from the GDB-11 database (~1600 molecules) MAE = 1.26 kcal/mol.

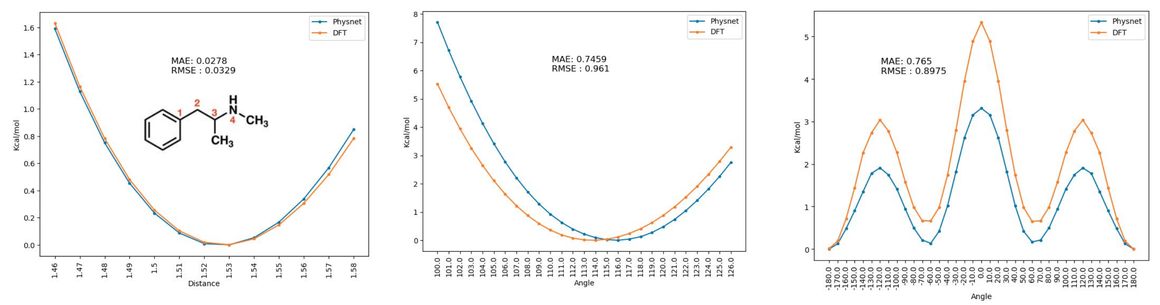

Fig 3:- Potential energy surface (in kcal/mol) corresponding to C-N bond stretching, C-C-C angle bending of Methamphetamine and C-C-C-C torsion angle rotation of n-decane calculated using PhysNet and DFT at ωB97X/6-31G(d) level of theory.

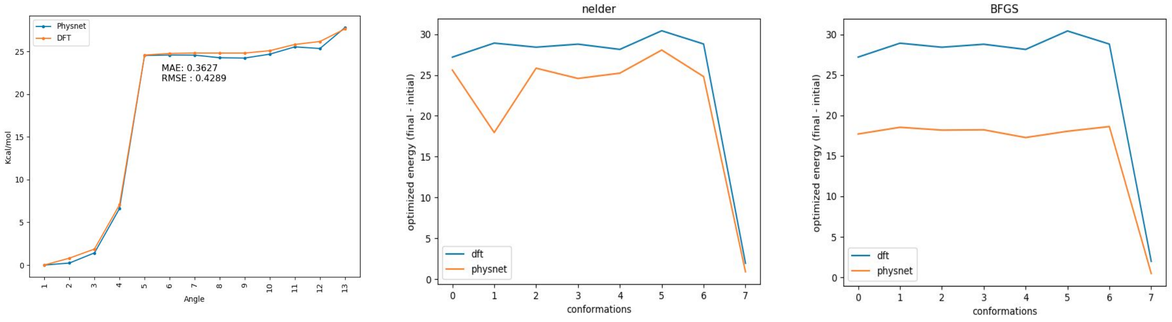

Fig 4:-Nelder mead and Broyden–Fletcher–Goldfarb–Shanno (BFGS) optimizer used for energy minimization of Methamphetamine using PhysNet compared to DFT at ωB97X/6-31G(d) level of theory.

CONCLUSION

- ★ NN predicts smooth and accurate Potential energy surfaces. Such a behavior is necessary for performing energy minimization, conformational analysis and force calculations.

REFERENCES

1. J. Chem. Theory Comput. 2019, 15, 3678−3693.
2. Chem. Sci.,2017, 8,3192–3203

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