Machine learned potential for Fe/P/C/O/H Systems

Vjeran Gomzi[a], *Iva Movre Šapić*[b], *Andrej Vidak*[b]
[a]*Faculty of electrical engineering and computing, University of Zagreb, Unska 3, Zagreb, Croatia*
[b]*Faculty of chemical engineering and technology, University of Zagreb, Marulićev trg 19, Zagreb, Croatia*

Vjeran.Gomzi@fer.unizg.hr

21 Ružičkini dani
DANAS ZNANOST – SUTRA INDUSTRIJA
9. – 11. rujna 2026. • Vukovar • Hrvatska

introduction

> Reactive force field approach applied in the ReaxFF package is a promising molecular dynamics (MD) method for modeling and simulation of chemical reactions at medium to large scales

> In $LiFePO_4$ based **batteries** lithium ferrophosphate is used as the cathode, while graphite is often used as the anode.

> **parameters** for **ReaxFF** MD for systems involving **Fe/P/C/O/H** atoms[1] are obtained and compared to physics - informed machine-learned potential on a consistent training set of 160 molecules

> The performance of the two approaches is evaluated by application on the same test set

software

> bash

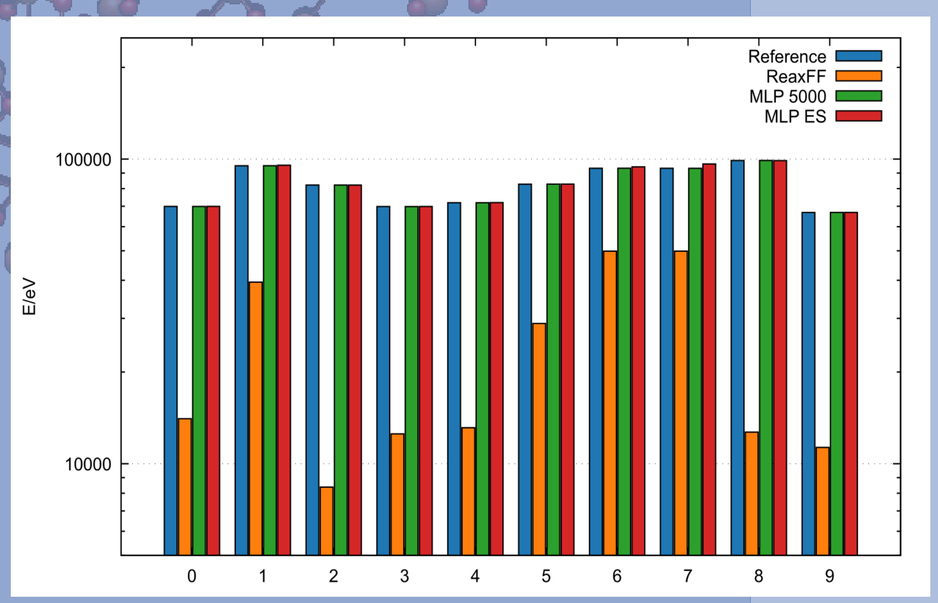
> Python + Optuna, Tensorlow

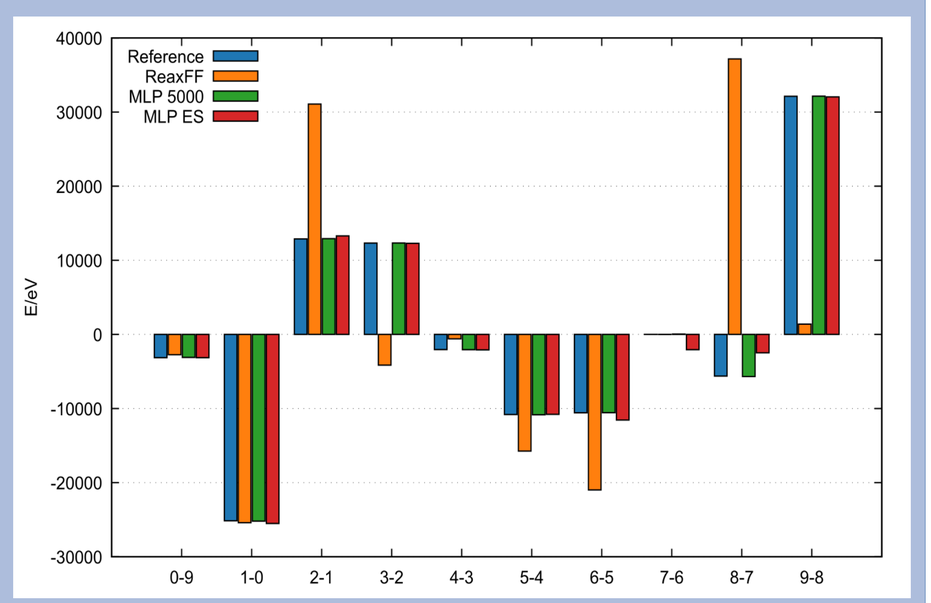
> Siesta

> Gaussian 09, Gaussian 16

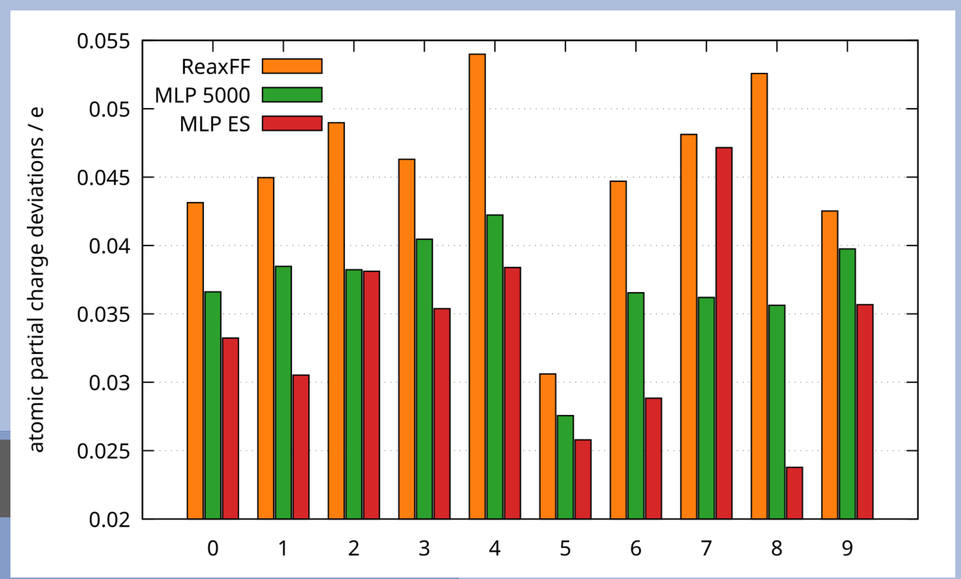
> HPC Supek SRCE

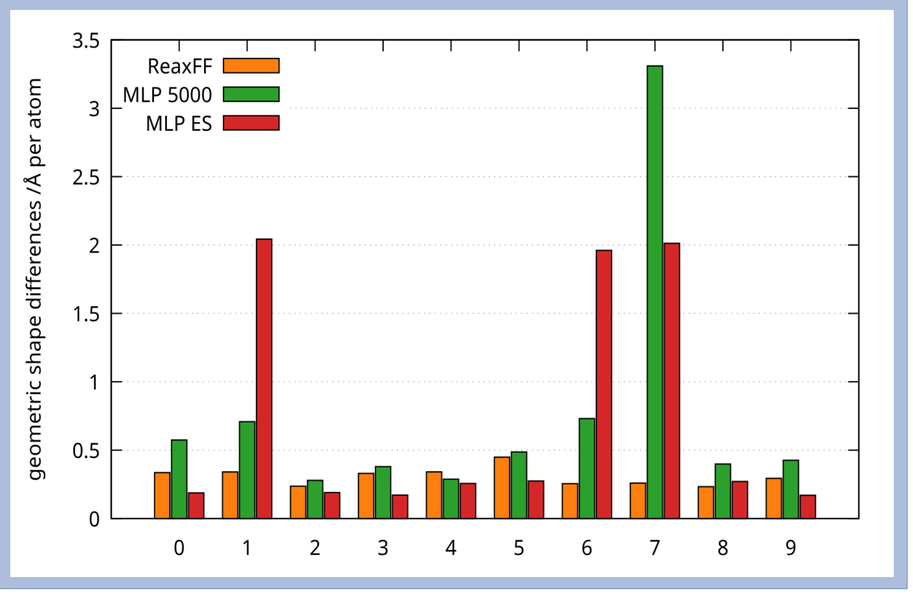
results





Energy, charge and geometry reproduction of DFT results by two methods and three approaches





methods

> collecting data (COD)[2]

> calculating DFT b3lyp/6-31+G

> A: MD FF optimization
>> choosing initial FF and parameters:
>> preparing inputs and running ReaxFF in a loop optimizing parameters

> B: MLP learning
>> building transformations for physics-informed ML parameters (phys. model)
>> layers and NN model construction

> evaluation and comparison: application of the model on the chosen set of new structures (10)

> differences and results above.

conclusions

> Energies and also their differences better reproduced by MLP

> Large parameter space hard to cover → ML better

> charges better reproduced by MLP also

> electronic properties better reproduced by physics-informed MLP!

> Structures better reproduced by MD

> Solutions?
>> possible different weights in previous steps (Reax initial FF)
>> better electronic model of MLP, but structure optimizer worse
>> long-distance (electronic contributions) not modeled well in MD, local bonding missing in MLP
>> training set mostly equilibrium! – MD has physical model of energy shape, MLP only infers it from data
>> suspicious DFT data (no optimization)

[1] V. Gomzi, I. Movre Šapić, A. Vidak, *Computation Chemistry Day*, Ruđer Bošković Institute, May 8-9 2026, Zagreb

[2] S. Gražulis, A. Daškevič, A. Merkys, *et al.*, *Nucleic Acids Res.* 2012, 40, D420−D427.