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Golam Mahmud Samdani 283 asked a question 2 days ago
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Resolved

MD Model Prediction #87

General

I'm trying to understand how molecular dynamics simulations are used to train machine learning models for predicting interatomic potentials—how do we ensure the model captures long-range interactions and remains accurate across different phases or defect structures?

1 0 77 29

Answers Comments
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Best

4

An instructor (Andre Schleife) endorsed this answer

Jahid Emon 1524 answered this question 2 days ago

To ensure machine-learned interatomic potentials trained on molecular dynamics data capture long-range interactions and remain accurate across phases or defects, researchers often include diverse training data that spans multiple configurations—equilibrium, strained, defected, and various phases. Models like MACE or NequIP can incorporate long-range physics through specialized architectures or explicit electrostatics. Additionally, techniques like active learning help adaptively sample regions where the model is uncertain, improving generalization to unseen structures.

Reply

2

An instructor (Andre Schleife) endorsed this answer

Wenwen LENG 59 answered this question 2 days ago

Traditional MLIPs (e.g., standard Deep Potential, MTP, GAP) typically rely on **local descriptors**, with only finite cutoff radius (e.g., 6–10 Å).I know that DeePMD group proposed an extension to their Deep Potential model by incorporating long-range electrostatics using a physically inspired approximation:

> The long-range Coulomb interaction between ions and valence electrons is modeled as interactions between **Gaussian charge distributions** placed at atomic and electronic centers.
>
> arXiv:2112.13327

This allows the model to:

- retain local symmetry-preserving neural networks,
- while adding an electrostatic baseline with distance-dependent interactions,
- and handle **heterogeneous charge distributions** more realistically.

In practice, if long-range interactions are important for your system, you'll need to:

- Use or extend a model that includes explicit electrostatics (e.g., DP-ZBL, DP-LR, PhysNet),
- Or combine MLIPs with **charge equilibration schemes** (QEq, HIPNN-QM9, etc.),
- And ensure your training set includes **diverse environments** (e.g., defects, interfaces, multiple phases) to promote generalizability.

Hope that helps.

1 reply Reply

Golam Mahmud Samdani 283 2 days ago

Thanks for explaining this nicely!

Reply