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Journal Club: E(3)-equivariant graph neural networks for data-efficient and accurate interatomic potential

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E(3)-equivariant graph neural networks for data-efficient and accurate interatomic potentials

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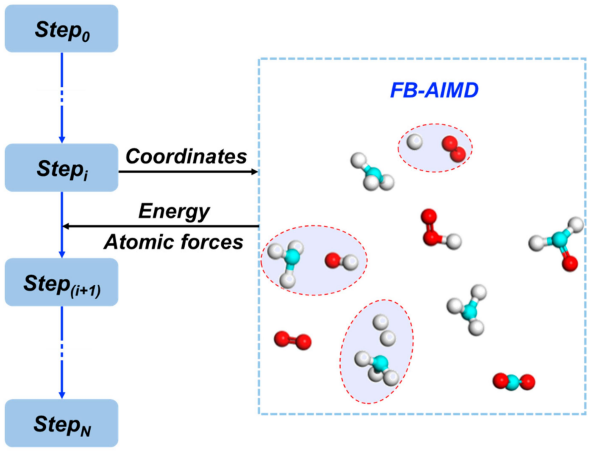
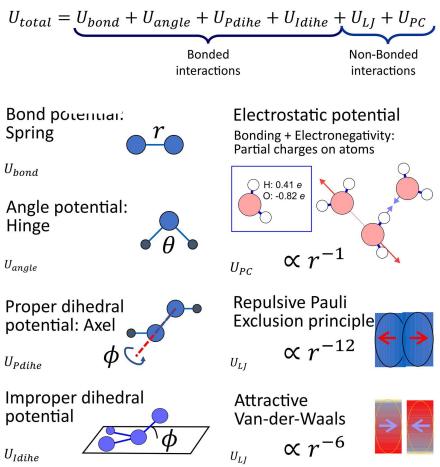
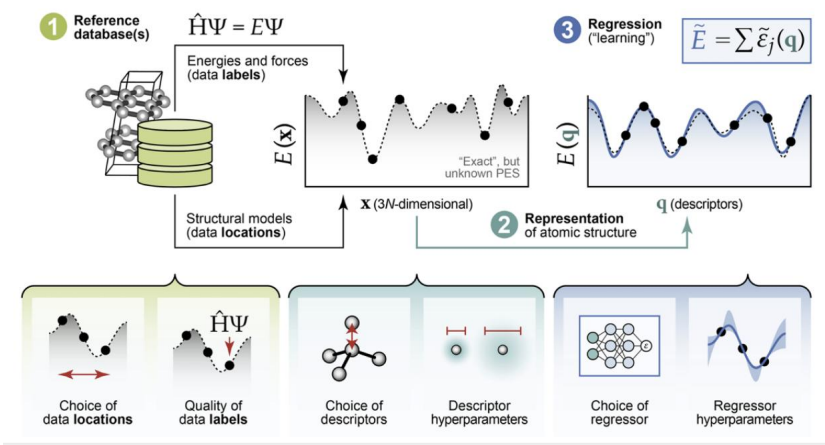
This work presents Neural Equivariant Interatomic Potentials (NequIP), an E(3)-equivariant neural network approach for learning interatomic potentials from ab-initio calculations for molecular dynamics simulations. While most contemporary symmetry-aware models use invariant convolutions and only act on scalars, NequIP employs E(3)-equivariant convolutions for interactions of geometric tensors, resulting in a more information-rich and faithful representation of atomic environments. The method achieves state-of-the-art accuracy on a challenging and diverse set of molecules and materials while exhibiting remarkable data efficiency. NequIP outperforms existing models with up to three orders of magnitude fewer training data, challenging the widely held belief that deep neural networks require massive training sets. The high data efficiency of the method allows for the construction of accurate potentials using high-order quantum chemical level of theory as reference and enables high-fidelity molecular dynamics simulations over long time scales.

Efficiency-Accuracy Trade-off in Molecular Dynamics

	Electronic Structure (DFT, etc.)	Classical Force Fields	Machine Learning Interatomic Potentials
Fast			( )
Accurate			( )
Big			( )







Machine Learning Interatomic Potentials (ML-IPs)

- **NN-IP Promise:** To learn high-fidelity potentials from *ab-initio* data while retaining favorable efficiency
- **NN-IP Bottleneck:** Typically require massive training sets (thousands to millions of reference structures).

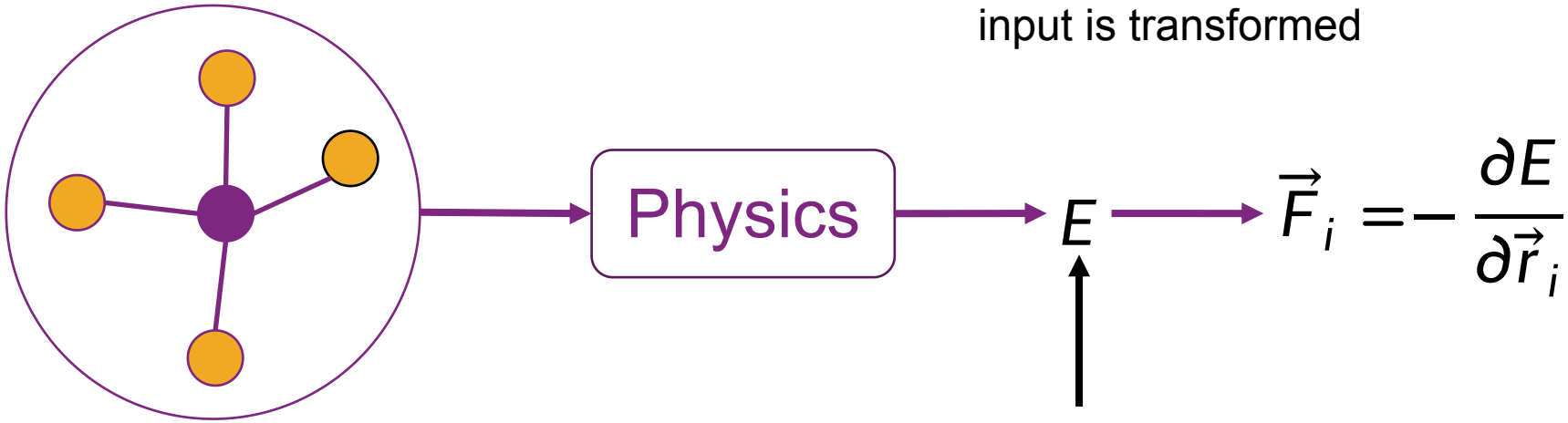
Neural Equivariant Interatomic Potentials (NequIP)

Achieves state-of-the-art accuracy while outperforming existing models with up to **three orders of magnitude fewer** training data.

Physical Symmetries

O(3)-equivariant model

Equivariant: internal features transform correspondingly when the input is transformed



Invariant: does not change

O(3)-invariant model

MD-17 Small Molecule Dynamics

Table 2 Energy and Force MAE for molecules on the revised MD-17 data set, reported in units of [meV] and [meV/Å], respectively, and a training budget of 1000 reference configurations.

Molecule		FCHL19	UNiTE	GAP	ANI	ACE	GemNet-(T/Q)	NequIP (l = 0)	NequIP (l = 1)	NequIP (l = 2)	NequIP (l = 3)
Aspirin	Energy	6.2	2.4	17.7	16.6	6.1	-	25.2	3.8	2.4	**2.3**
	Forces	20.9	**7.6**	44.9	40.6	17.9	9.5	42.2	12.6	8.5	8.2
Azobenzene	Energy	2.8	1.1	8.5	15.9	3.6	-	20.3	1.1	0.8	**0.7**
	Forces	10.8	4.2	24.5	35.4	10.9	-	34.4	4.5	3.3	**2.9**
Benzene	Energy	0.3	0.07	0.75	3.3	**0.04**	-	3.2	0.09	0.06	**0.04**
	Forces	2.6	0.73	6.0	10.0	0.5	0.5	10.3	0.4	0.4	**0.3**
Ethanol	Energy	0.9	0.62	3.5	2.5	1.2	-	2.0	1.0	0.5	**0.4**
	Forces	6.2	3.7	18.1	13.4	7.3	3.6	11.9	6.5	3.5	**2.8**
Malonaldehyde	Energy	1.5	1.1	4.8	4.6	1.7	-	4.4	1.6	0.9	**0.8**
	Forces	10.2	6.6	26.4	24.5	11.1	6.6	23.2	10.3	5.9	**5.1**
Naphthalene	Energy	1.2	0.46	3.8	11.3	0.9	-	14.7	0.4	0.3	**0.2**
	Forces	6.5	2.6	16.5	29.2	5.1	1.9	20.6	2.1	1.4	**1.3**
Paracetamol	Energy	2.9	1.9	8.5	11.5	4.0	-	17.5	2.1	**1.4**	**1.4**
	Forces	12.2	7.1	28.9	30.4	12.7	-	33.6	9.3	**5.9**	**5.9**
Salicylic acid	Energy	1.8	0.73	5.6	9.2	1.8	-	11.4	1.0	0.8	**0.7**
	Forces	9.5	3.8	24.7	29.7	9.3	5.3	29.8	5.7	4.2	**4.0**
Toluene	Energy	1.6	0.45	4.0	7.7	1.1	-	9.7	0.5	**0.3**	**0.3**
	Forces	8.8	2.5	17.8	24.3	6.5	2.2	26.6	2.6	1.8	**1.6**
Uracil	Energy	0.6	0.58	3.0	5.1	1.1	-	10.0	0.6	**0.4**	**0.4**
	Forces	4.2	3.8	17.6	21.4	6.6	3.8	26.0	4.1	**2.9**	3.1

For GemNet, the best result out of the T/Q versions is presented. For FCHL19, the best results between energy-only, force-only and joint force and energy training are presented. For UNiTE, we compare to the "direct-learning" results reported in[26].
Best results are marked in bold.

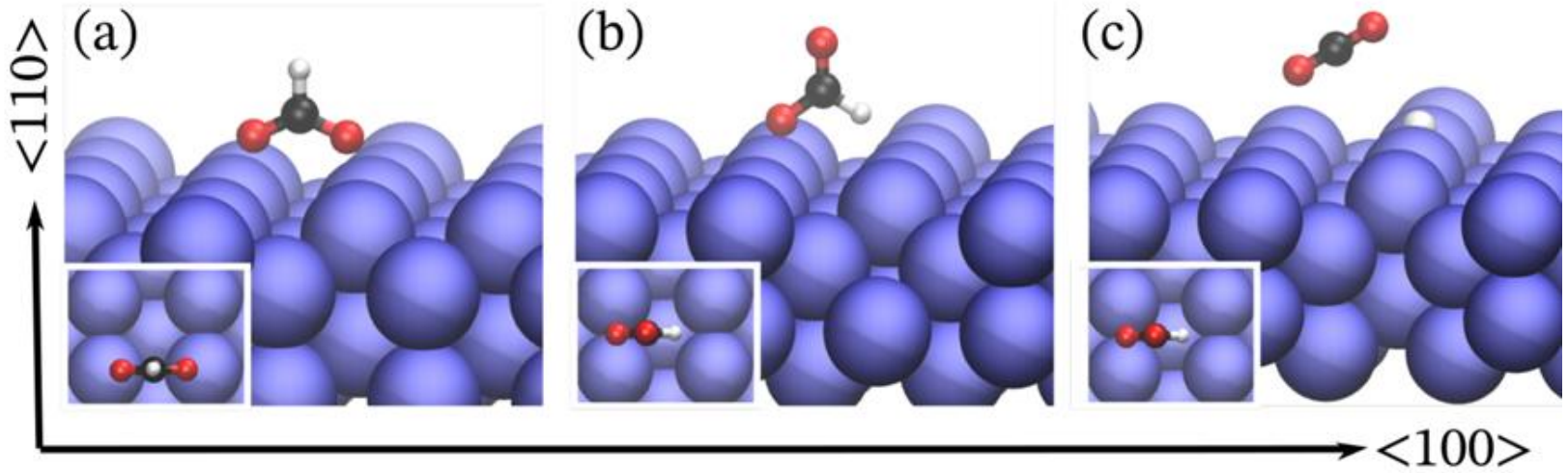
Liquid Water and Ice Dynamics

Table 3 RMSE of energies and forces on liquid water and the three ices in units of [meV/molecule] and [meV/Å], with energy errors normalized by the number of molecules in the system.

System		NequIP, a)	NequIP, b)	NequIP, c)	DeepMD
Liquid Water	Energy	-	1.6	1.7	1.0
	Forces	11.9	49.4	11.6	40.4
Ice Ih (b)	Energy	-	2.5	4.3	0.7
	Forces	10.2	55.8	9.9	43.3
Ice Ih (c)	Energy	-	3.9	10.2	0.7
	Forces	12.0	27.7	11.7	26.8
Ice Ih (d)	Energy	-	2.6	12.7	0.8
	Forces	9.8	23.2	9.5	25.4

Note that the NequIP models were trained on <0.1% of the training data of DeepMD. NequIP model (a) refers to loss function weighting $\lambda_F = 1, \lambda_E = 0$, model (b) to $\lambda_F = 100, \lambda_E = 1$, and model c) to $\lambda_F = 100,000, \lambda_E = 1$.

Heterogeneous Catalysis of Formate Dehydrogenation



Average force MAE: 38.4 meV/Å
Energy MAE: 0.50 meV/atom

Lithium Phosphate Amorphous Glass Formation

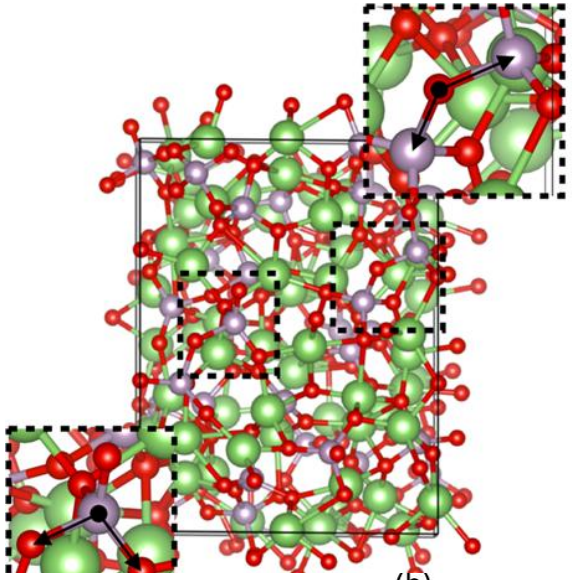
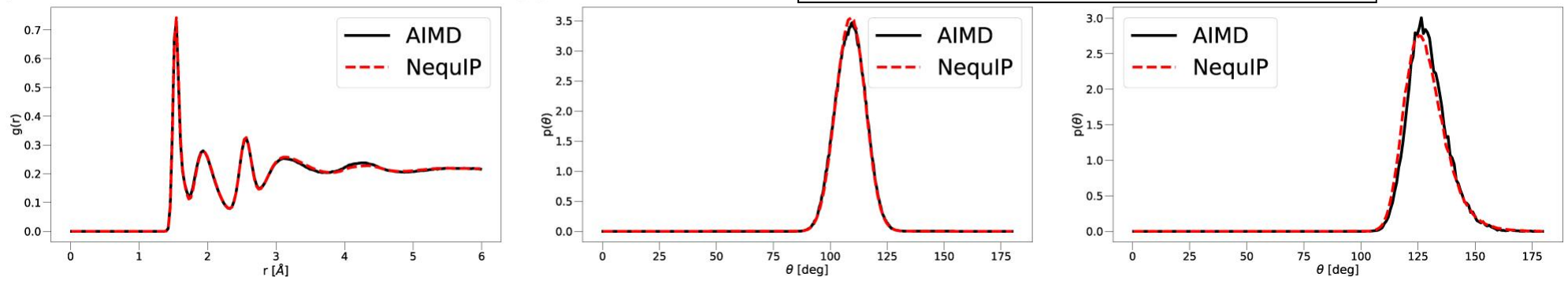


Table 4 NequIP E/F MAE/RMSE for LiPS and $Li_4P_2O_7$ for different data set sizes in units of [meV/Å] and [meV/atom].

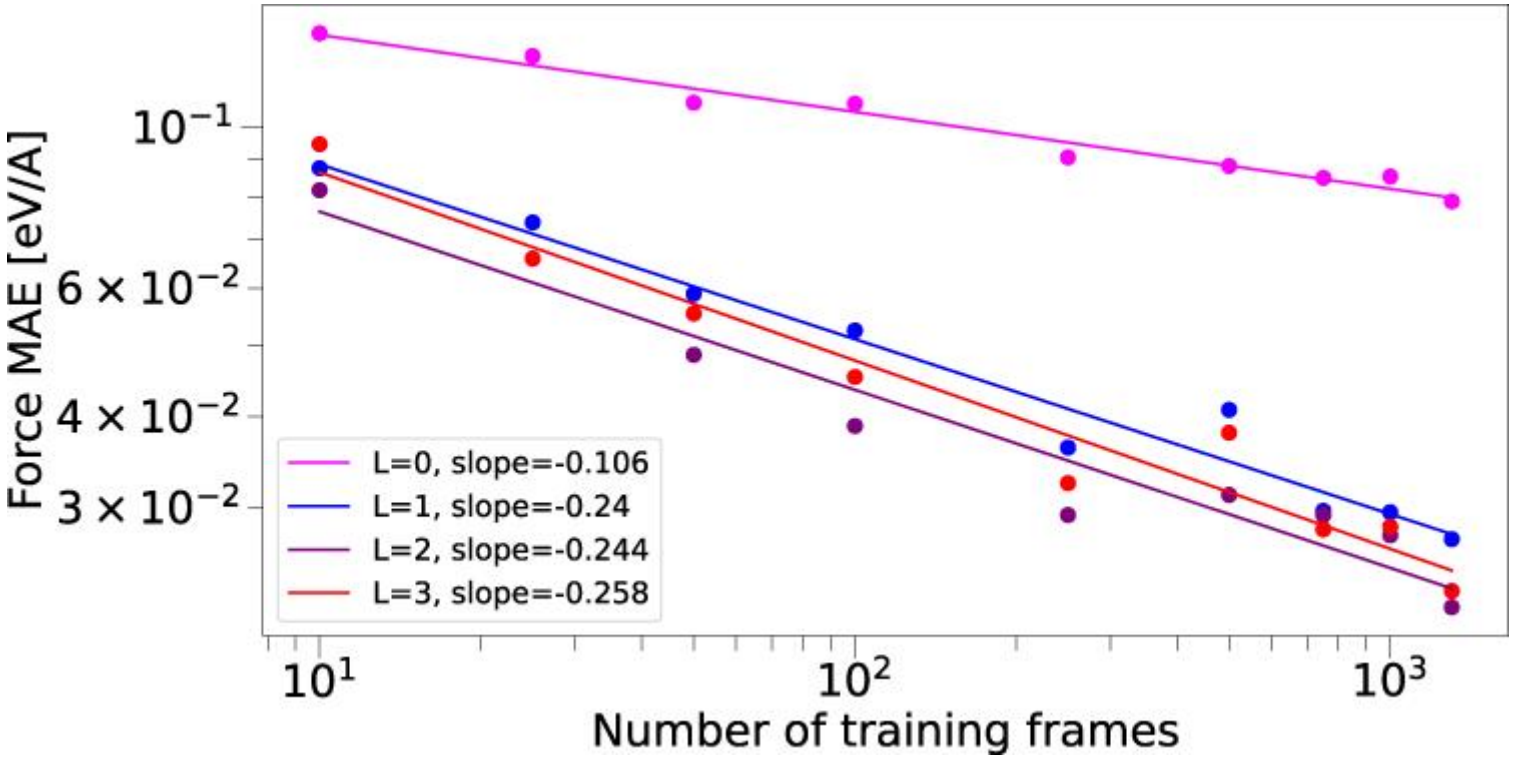
System	Data set size		MAE	RMSE
LiPS	10	Energy	2.03	2.54
		Forces	97.8	132.4
LiPS	100	Energy	0.44	0.56
		Forces	25.8	35.0
LiPS	1000	Energy	0.12	0.15
		Forces	7.7	10.8
LiPS	2500	Energy	0.08	0.10
		Forces	4.7	6.5
$Li_4P_2O_7$, melt	1000	Energy	0.4	0.8
		Forces	34.0	59.5
$Li_4P_2O_7$, quench	1000	Energy	0.5	0.5
		Forces	21.3	34.9

The model for $Li_4P_2O_7$ was trained exclusively on structures from the melted trajectory. The reported test errors for the melt are computed on the remaining set of structures from the full melt trajectory; errors for the quench are computed on the full quench trajectory.

(a) (b)



Data Efficiency



Conclusions

- NequIP is an energy-conserving interatomic potential built on E(3)-equivariant convolutions.
- Equivariant convolutions over geometric tensors provide a more faithful representation of the atomic environment.
- Achieves state-of-the-art accuracy on MD-17 and diverse extended systems.
- Demonstrates outstanding data efficiency, making it possible to use limited, high-quality *ab-initio* data for model training.

Thank You