

Supplementary Information

EAC-Net: Predicting real-space charge density via equivariant atomic contributions

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Supplementary Tables and Figures

Table 1: Model Performance Train Parameters

Parameter	a-Si	Al surface	Al-Mg	Water	Fe
Num params	0.37M~0.81M	0.28M~0.62M	0.94M~2.84M	0.28M~0.62M	0.94M
Training steps	150000	150000	250000	150000	200000
Atom feature len	24	24	36	24	36
Max Atom L	3/4/5/6	2/3/4	2/3/4/5	2/3/4/5	4
Num atom convs	3	3	4	3	4
Grid feature len	24	24	36	24	36
Max Grid L	3/4/5/6	2/3/4	2/3/4/5	2/3/4/5	4
Num edge update	2	3	2	2	2
Atom cutoff	4.0	4.0	4.0	4.0	4.0
Grid cutoff	6.0	6.0	6.0	6.0	6.0
Scalar neurons	240	240	240,240	240	240,240
Weight neurons	240	240	240	240	240
Weight type	MLP+S	MLP+S	MLP+S	MLP+S	MLP+S
Cat features	All	All	r, B	All	r, B
Batch size	50	50	50	50	50
Start learning rate	0.003	0.003	0.003	0.003	0.003
End learning rate	1e-8	1e-8	1e-7	1e-8	1e-5

Detailed network configuration and accuracy metrics for each test system.

Table 2: EAC-mp Large-Scale Training Configuration

Category	Parameters
Dataset Specifications	
Data source	Materials Project (MP)
Training frames num	48,183
Test frames num	50,000
Probes per frame	5000
Probes sample method	Random
Hardware Configuration	
GPUs	$2 \times$ NVIDIA RTX A6000 (48GB)
Precision	FP32
Model Architecture	
Num params	3083892
Atom feature len	36
Max Atom L	5
Num atom convs	4
Grid feature len	36
Max Grid L	5
Num edge update	2
Atom cutoff	4.0
Grid cutoff	6.0
Scalar neurons	200,200
Weight neurons	200
Weight type	MLP+S
Cat features	All
Activation function	SiLU
Training Protocol	
Batch size	$25\text{frames} \times 30\text{probes}$
Training steps	600,000
Initial Learning Rate	$1e-3$
Final Learning Rate	$2.3e-5$
Learning rate schedule	Exponential Decay
Optimizer	Adam

Validation Loss Curve over Training Steps for EAC-mp Large-Scale Training.

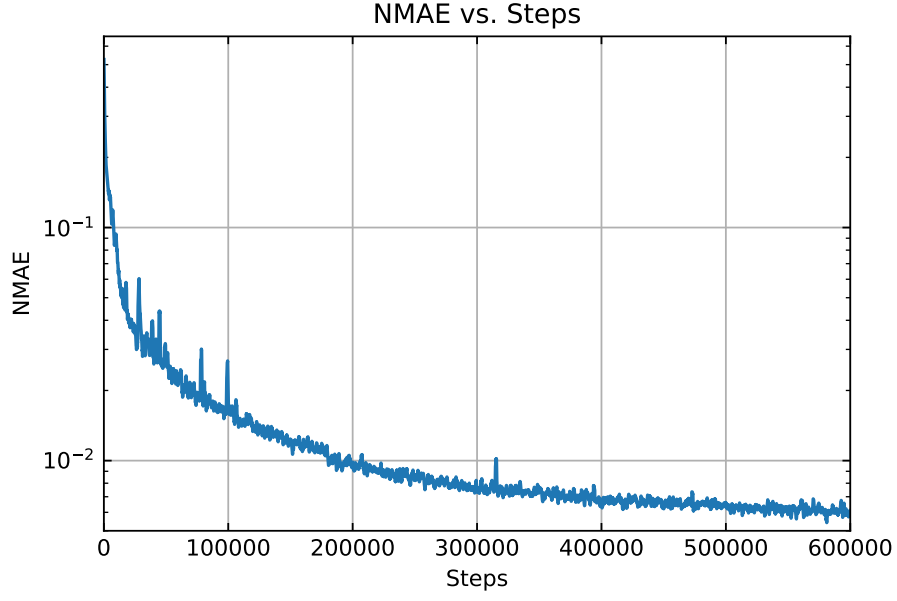


Figure 1: Validation Loss Curve over Training Steps.

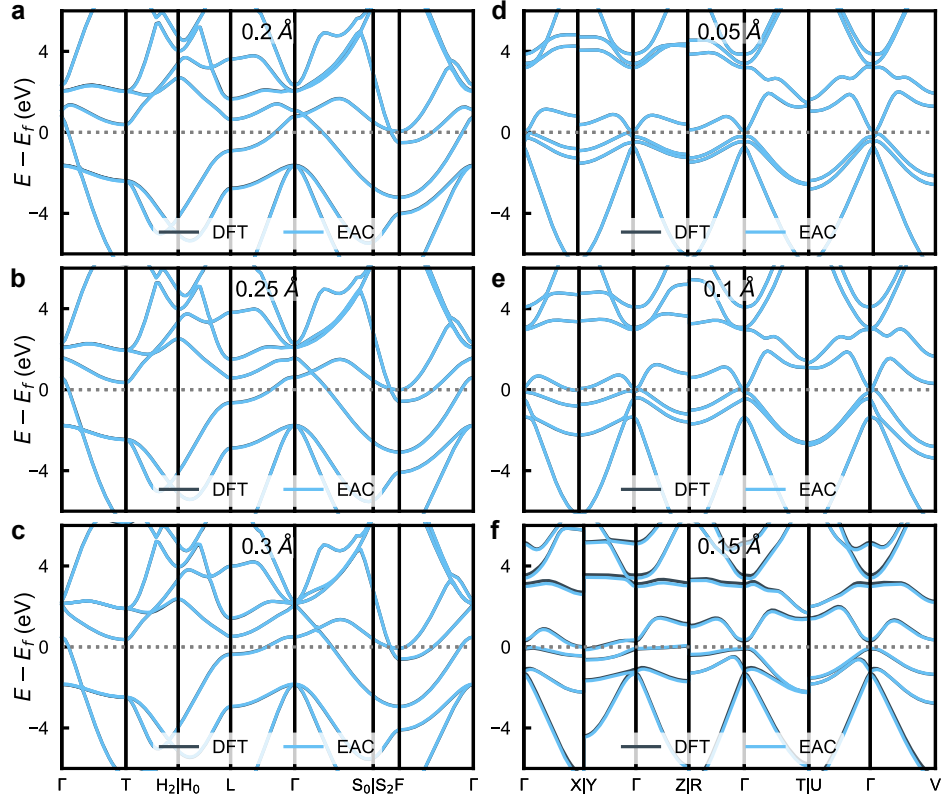


Figure 2: **a-c**, The band comparison between DFT and EAC results under different atomic displacement. **d-f**, The band comparison between DFT and EAC results under different perturbations on atoms and lattices.

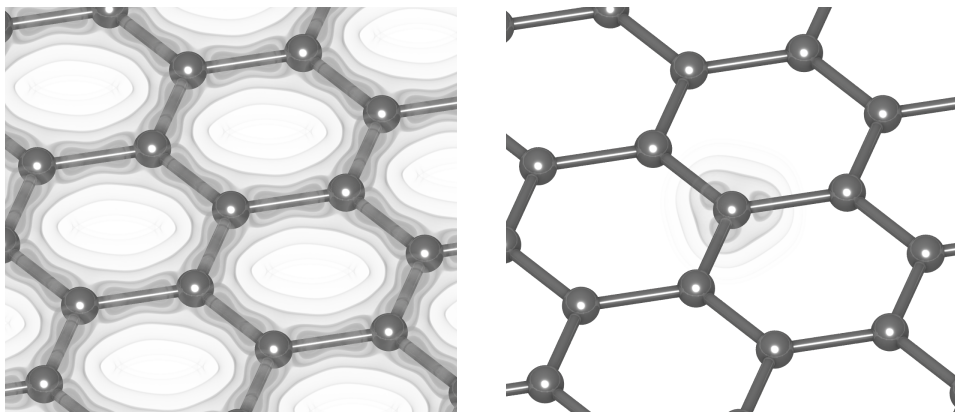


Figure 3: The total (left) and atomic (right) charge density inside a graphite layer.