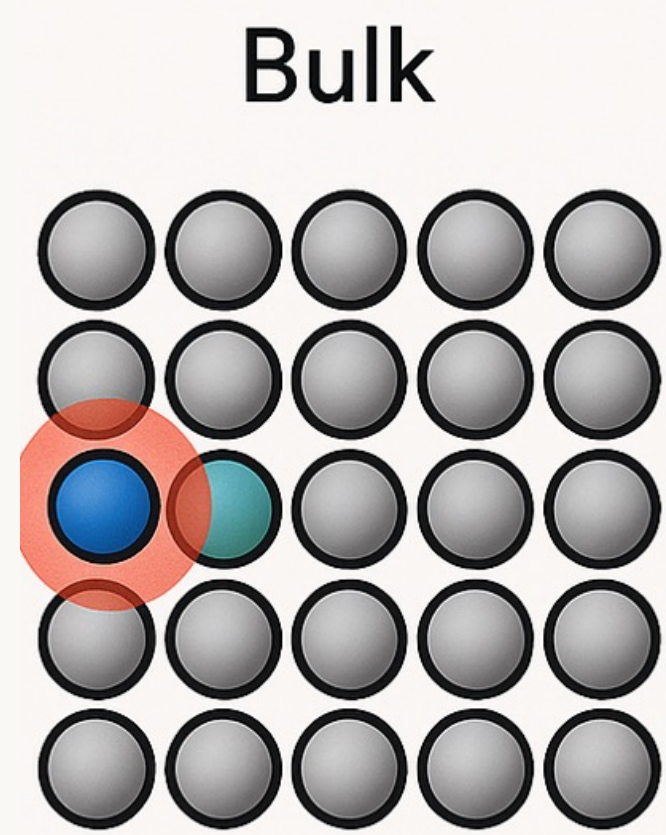
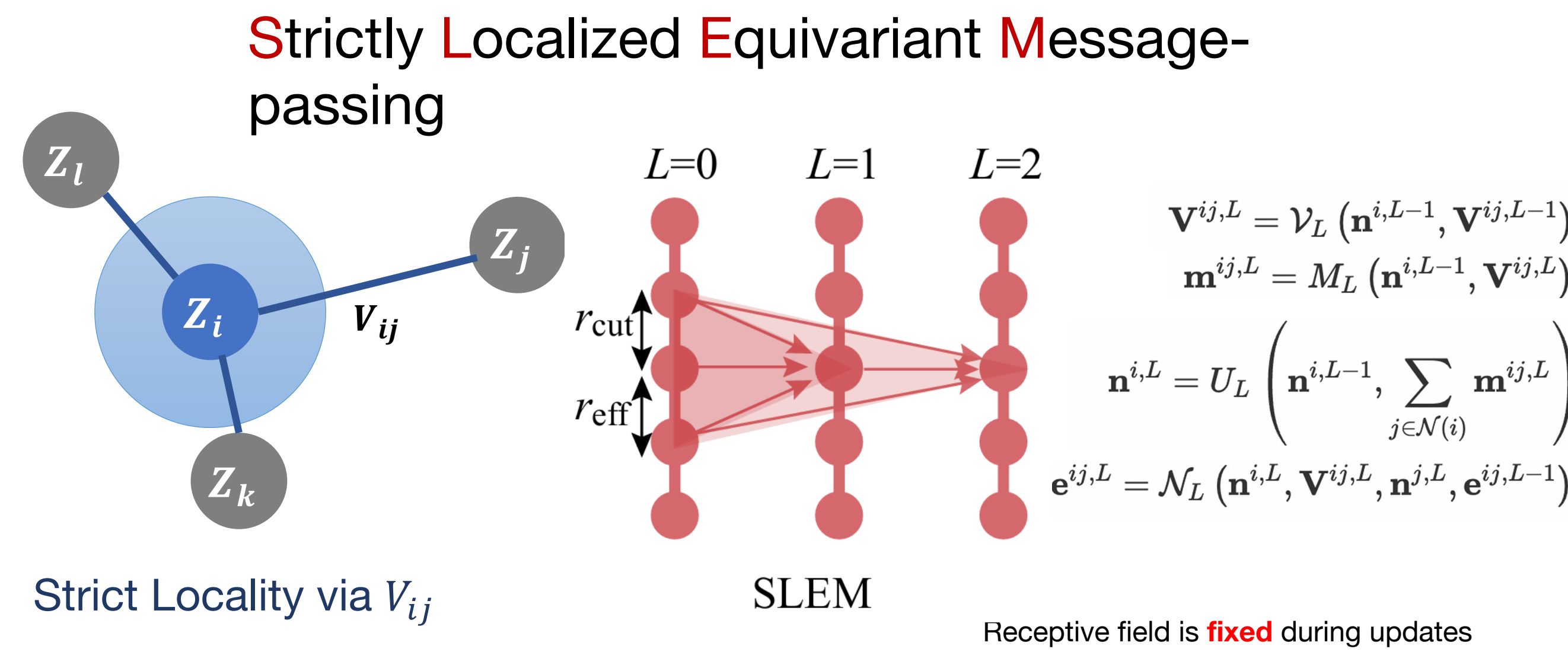
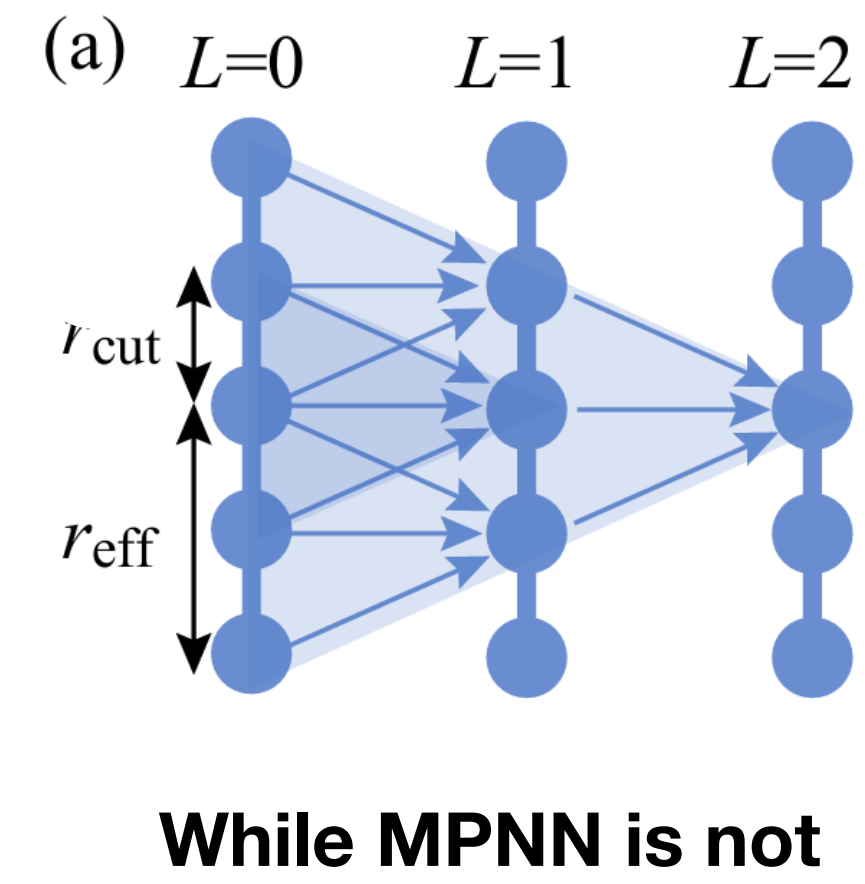
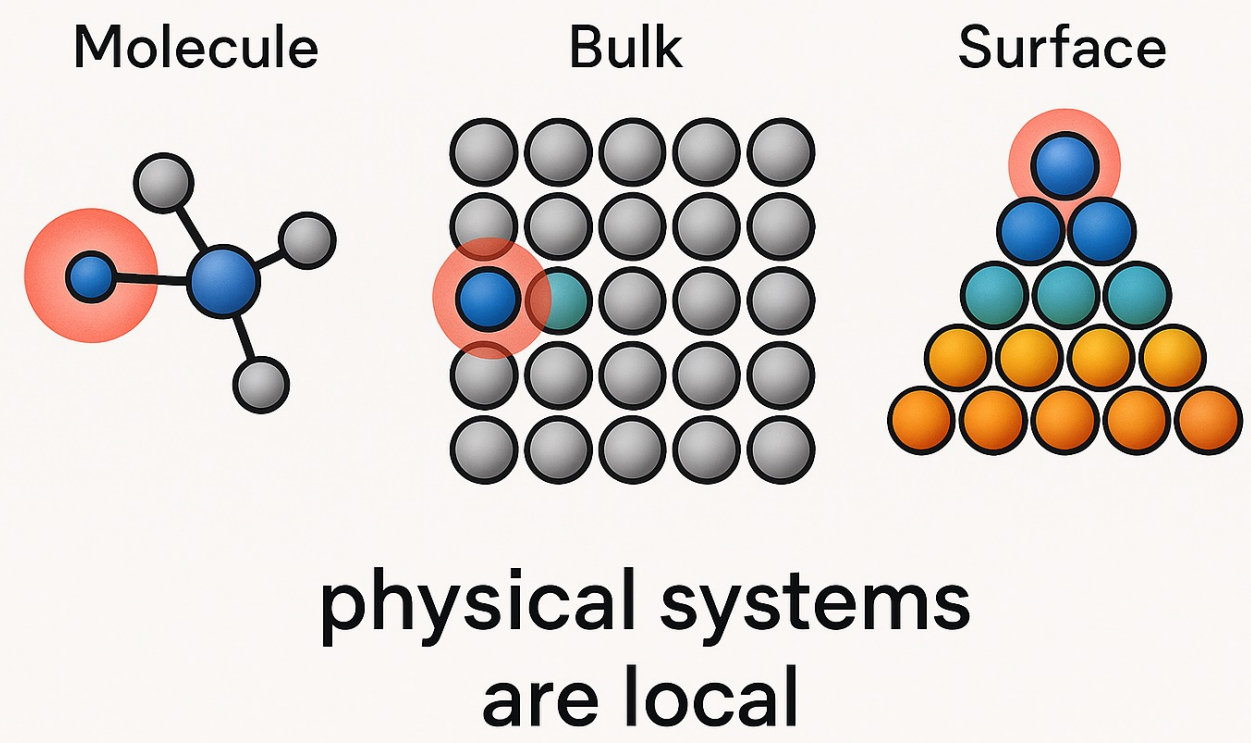


Learning Local Equivariant Representations for Quantum Operators

Spotlight



Authors: Zhanghao Zhouyin, Zixi Gan, MingKang Liu, Shishir Kumar Pandey, Linfeng Zhang Qiangqiang Gu[#]



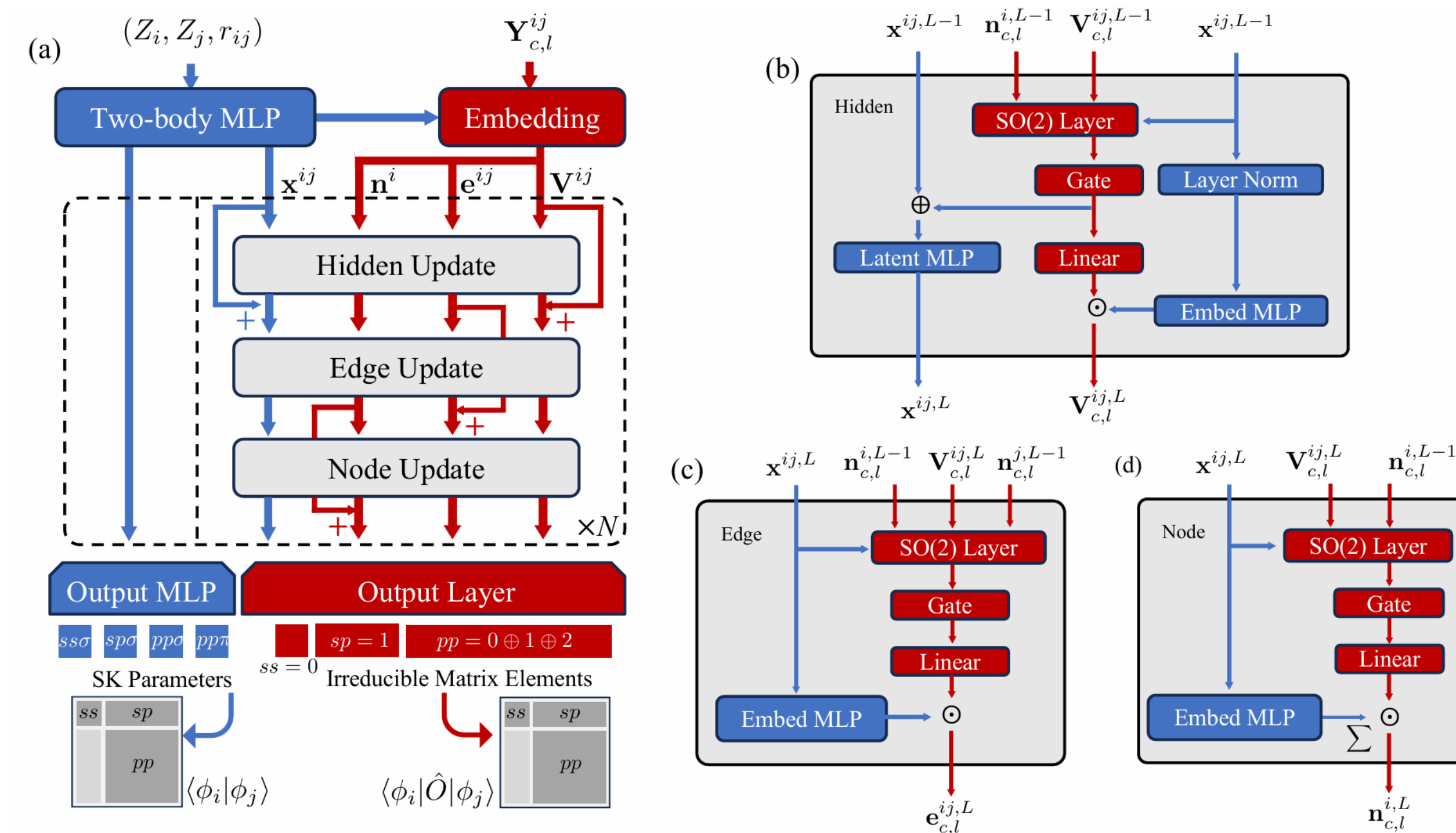
Electrical neutralization
#electrons = #protons in each direction

$$-\frac{Z_I}{r - R_I} + \int \frac{n_I(r' - R_I)}{|r - r'|} dr' \approx -\frac{Z_I}{|r - R_I|} + \frac{Z_I}{|r - R_I|} = 0$$

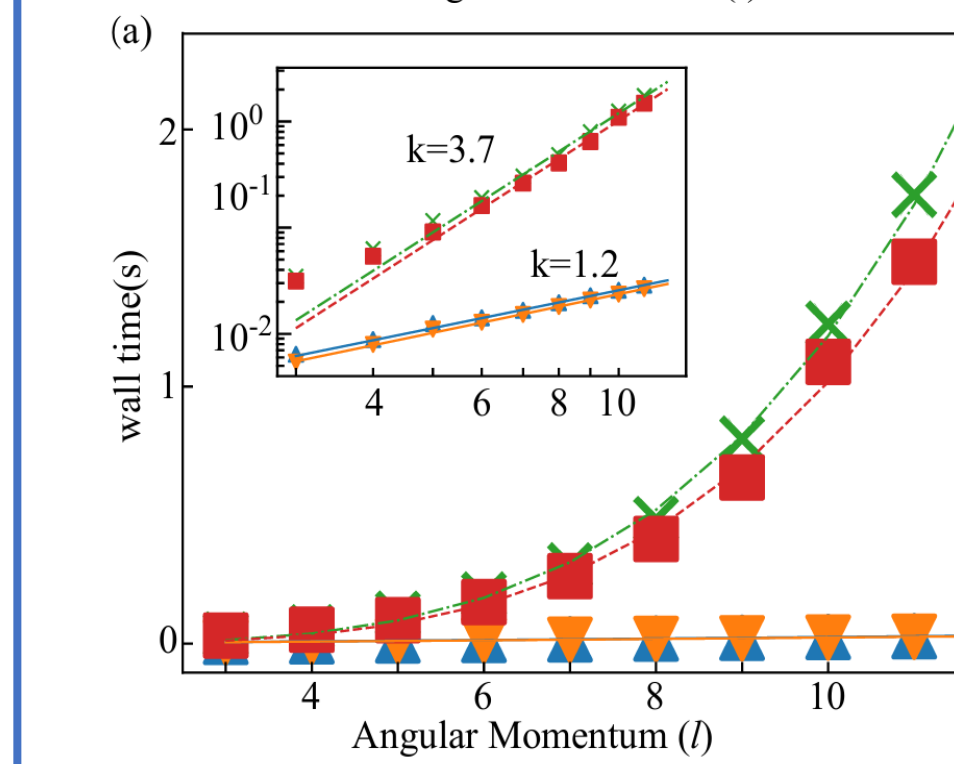
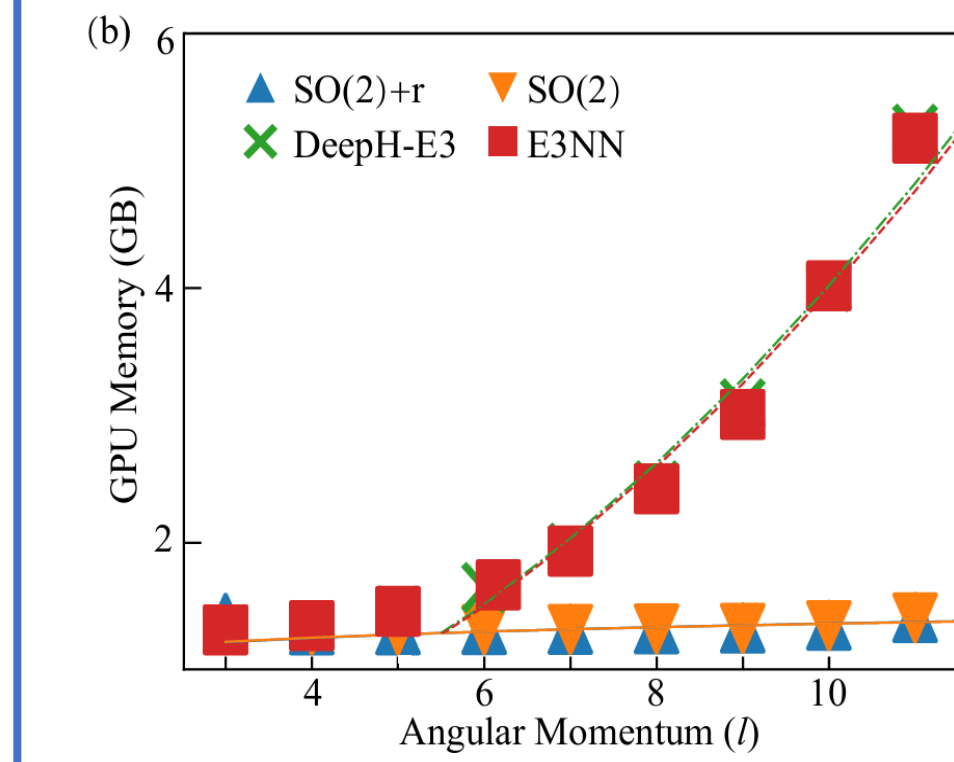
Screening Effect
Typical Screening Radius:

Diamond: 2.76 a.u Sil: 4.28 a.u. and Ge: 4.71 a.u.

A Strictly local will maintain the many-body interactive updates of MPNN like framework is beneficial to physical quantities predictions.



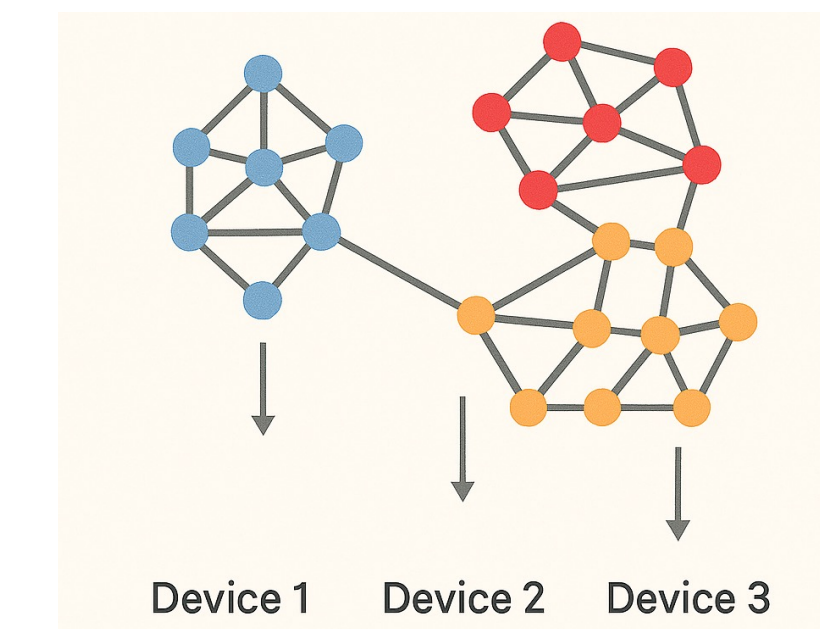
Efficiency



SLEM overlap prediction

Materials	Silicon	GaN	HfO ₂
MAE	5.6e-5	4.7e-5	6.3e-5

Fitting Overlap with **1.4% of increase of cost**



Parallelizability

Transferability

MoS ₂					
Partition	100%	80%	60%	40%	20%
SLEM	0.34	0.37	0.39	0.37	0.37
DeePH-E3	0.46	0.72	0.84	1.03	1.46
Graphene					
Partition	100%	80%	60%	40%	20%
SLEM	0.26	0.26	0.27	0.21	0.26
DeePH-E3	0.40	0.30	0.33	0.36	0.60

Sota Accuracy across basis angular momentum

Systems with LCAO-basis up to d -orbitals					
Material	SLEM (0.7M)	SLEM (4.5M)	DeepH-E3 (1.0 M)	DeepH-E3 (4.5M)	HamGNN (2.8M)
MoS ₂	0.34	0.14	0.46	0.55	1.20
Graphene	0.26	0.14	0.40	0.28	0.35
Si(300K)	0.10	0.07	0.16	0.10	0.19

Systems with LCAO-basis up to f and g -orbitals

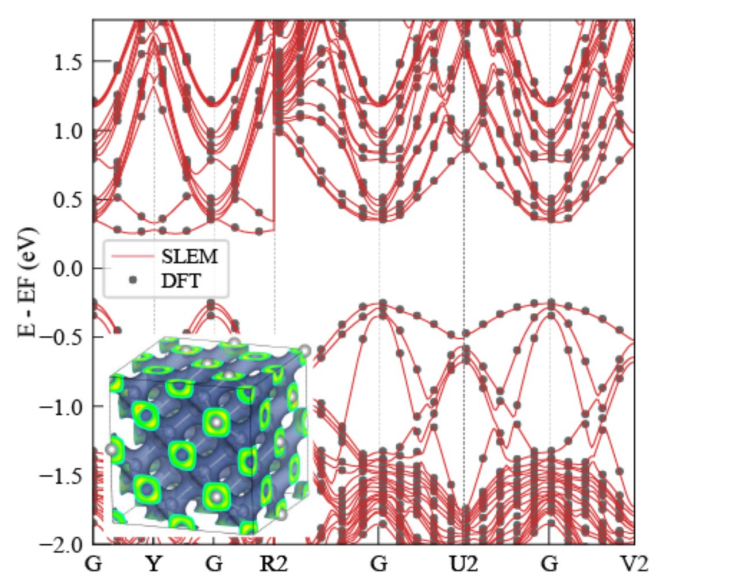
Material	SLEM (1.7M)	DeepH-E3 (1.9M)
GaN	0.21	0.87
HfO ₂	0.28	-

Sota Accuracy on molecules with semi-local variant LEM

QH-9 dataset benchmark				
Method	all	H[10 ⁻⁶ E _h]	diag	D all
LEM	56.57	44.86	155.24	0.0219
QHnet	83.22	80.26	135.63	0.0643

SLEM density matrix model			
Materials	Silicon	GaN	HfO ₂
MAE	8.9e-5	2.3e-5	3.9e-5

Fitting Density Matrix and used to do one-shot DFT SCF calculation.

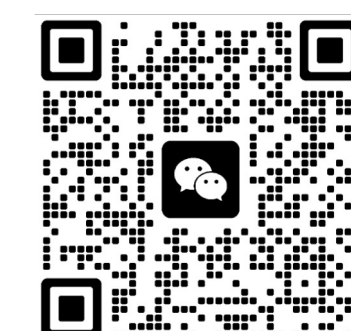


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Repo: **DeePTB**

<https://github.com/deepmodeling/DeePTB>

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