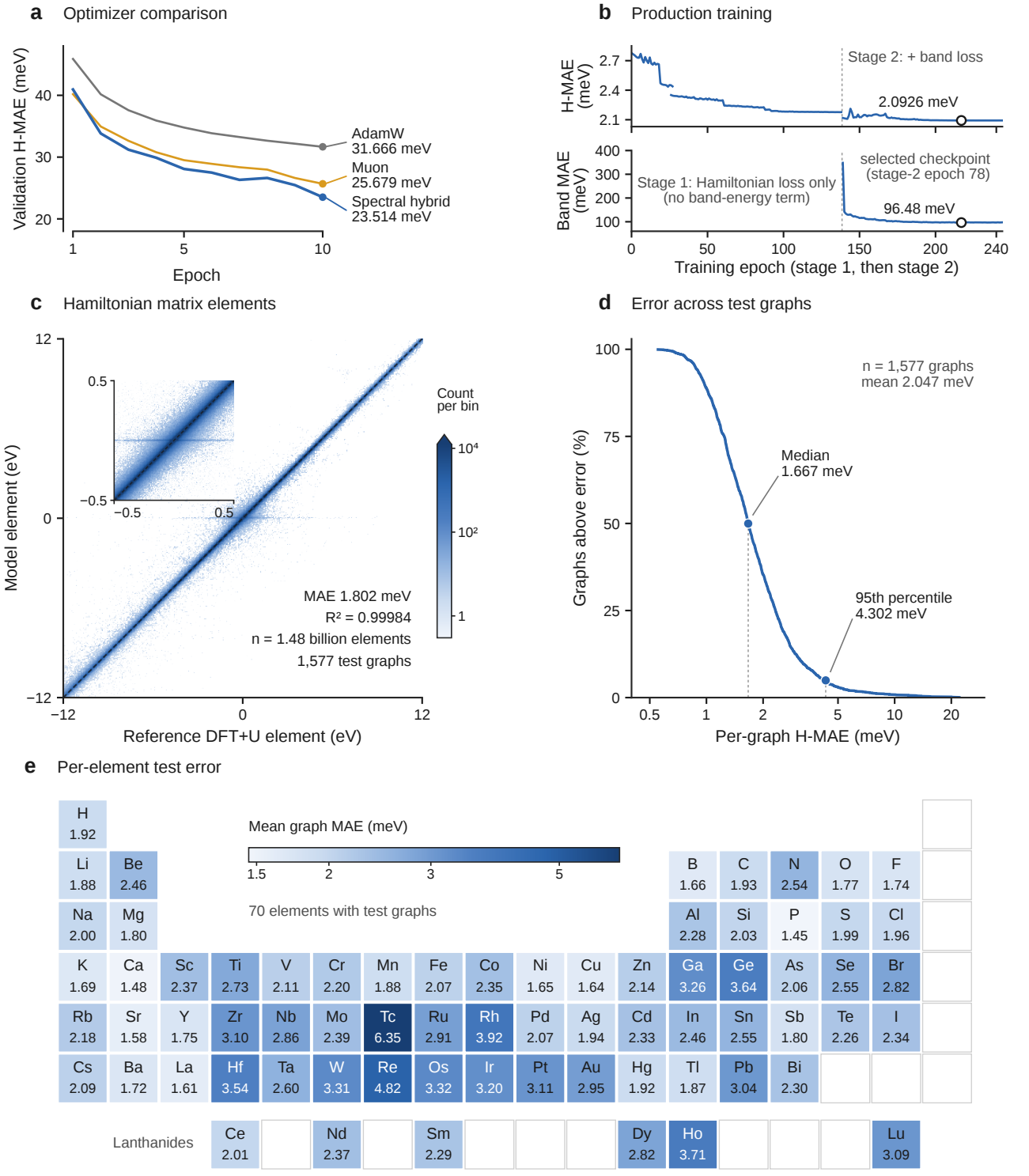

a
Optimizer comparison
Validation H-MAE (meV)
40
30
20
1
5
10
Epoch
AdamW
31.666 meV
Muon
25.679 meV
Spectral hybrid
23.514 meV
b
Production training
H-MAE (meV)
2.7
2.4
2.1
Stage 2: + band loss
2.0926 meV
Band MAE (meV)
400
300
200
100
Stage 1: Hamiltonian loss only
(no band-energy term)
selected checkpoint
(stage-2 epoch 78)
96.48 meV
0
50
100
150
200
240
Training epoch (stage 1, then stage 2)
c
Hamiltonian matrix elements
Model element (eV)
12
0
−12
0.5
−0.5
−0.5
0.5
Count per bin
10⁴
10²
1
MAE 1.802 meV
R² = 0.99984
n = 1.48 billion elements
1,577 test graphs
−12
0
12
Reference DFT+U element (eV)
d
Error across test graphs
Graphs above error (%)
100
75
50
25
0
n = 1,577 graphs
mean 2.047 meV
Median
1.667 meV
95th percentile
4.302 meV
0.5
1
2
5
10
20
Per-graph H-MAE (meV)
e
Per-element test error
Mean graph MAE (meV)
1.5
2
3
5
70 elements with test graphs
H 1.92
Li 1.88
Be 2.46
B 1.66
C 1.93
N 2.54
O 1.77
F 1.74
Na 2.00
Mg 1.80
Al 2.28
Si 2.03
P 1.45
S 1.99
Cl 1.96
K 1.69
Ca 1.48
Sc 2.37
Ti 2.73
V 2.11
Cr 2.20
Mn 1.88
Fe 2.07
Co 2.35
Ni 1.65
Cu 1.64
Zn 2.14
Ga 3.26
Ge 3.64
As 2.06
Se 2.55
Br 2.82
Rb 2.18
Sr 1.58
Y 1.75
Zr 3.10
Nb 2.86
Mo 2.39
Tc 6.35
Ru 2.91
Rh 3.92
Pd 2.07
Ag 1.94
Cd 2.33
In 2.46
Sn 2.55
Sb 1.80
Te 2.26
I 2.34
Cs 2.09
Ba 1.72
La 1.61
Hf 3.54
Ta 2.60
W 3.31
Re 4.82
Os 3.32
Ir 3.20
Pt 3.11
Au 2.95
Hg 1.92
Tl 1.87
Pb 3.04
Bi 2.30
Lanthanides
Ce 2.01
Nd 2.37
Sm 2.29
Dy 2.82
Ho 3.71
Lu 3.09