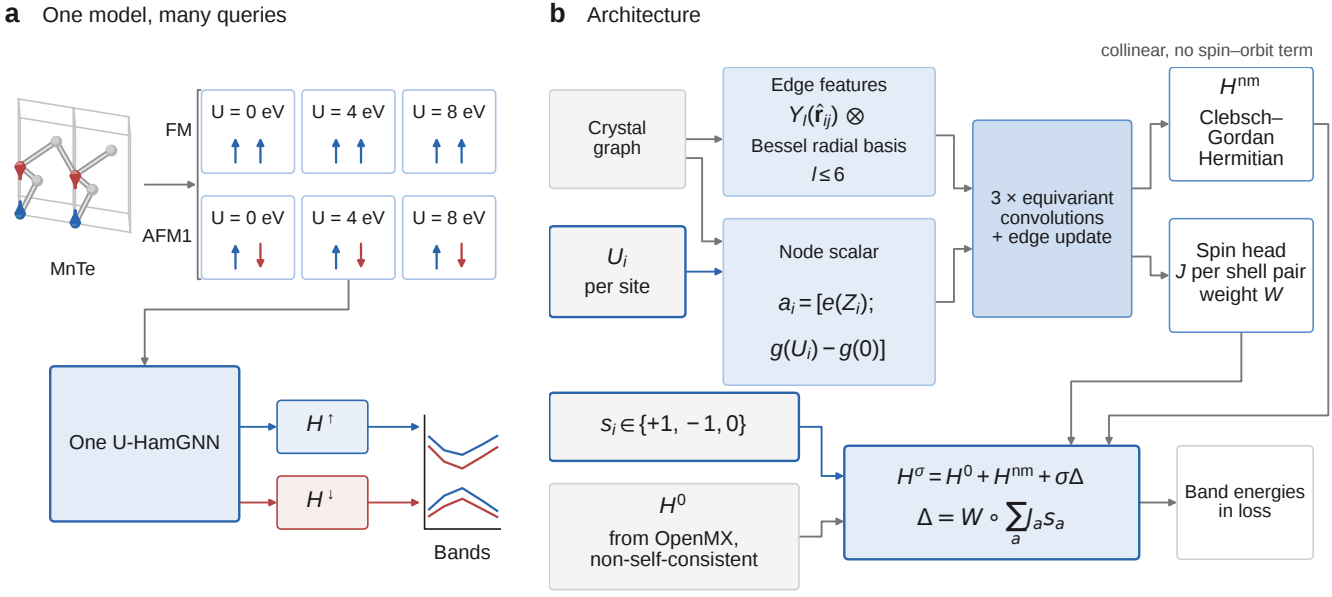

a
One model, many queries
MnTe
FM
AFM1
U = 0 eV
U = 4 eV
U = 8 eV
U = 0 eV
U = 4 eV
U = 8 eV
One U-HamGNN
$H^{\uparrow}$
$H^{\downarrow}$
Bands
b
Architecture
collinear, no spin–orbit term
Crystal graph
Edge features
$Y_l(\hat{\mathbf{r}}_{ij}) \otimes$
Bessel radial basis
$l \le 6$
U_i
per site
Node scalar
$a_i = [e(Z_i);$
$g(U_i) - g(0)]$
3 × equivariant convolutions + edge update
H^{nm}
Clebsch–Gordan Hermitian
Spin head
J per shell pair
weight W
$s_i \in \{+1, -1, 0\}$
H^0
from OpenMX, non-self-consistent
$H^{\sigma} = H^0 + H^{nm} + \sigma\Delta$
$\Delta = W \circ \sum_a J_a s_a$
Band energies in loss