#### Complete Buckingham Potential (Thermal MD)

#### Parameterization

# MFO\_Buckingham.in  
pair\_style buck/coul/long 12.0  
#---- Atomic Charges (Formal) ----   
set type 1 charge +2 # Mn²⁺ (tetrahedral A-site)  
set type 2 charge +3 # Fe³⁺ (octahedral B-site)  
set type 3 charge -2 # O²⁻   
  
#---- Pair Coefficients ----   
pair\_coeff 1 1 0.0 1.0 0.0 # Mn-Mn (Coulomb only)  
pair\_coeff 1 2 0.0 1.0 0.0 # Mn-Fe (Coulomb only)  
pair\_coeff 2 2 0.0 1.0 0.0 # Fe-Fe (Coulomb only)  
pair\_coeff 1 3 649.1 0.3399 0.0 # Mn-O (≈Fe²⁺-O in FO-Buck-3)  
pair\_coeff 2 3 1414.6 0.3128 0.0 # Fe-O (FO-Buck-3 Fe³⁺-O)  
pair\_coeff 3 3 9547.96 0.2192 32.0 # O-O (FO-Buck-3)  
  
#---- Long-Range Electrostatics ----   
kspace\_style pppm 1e-5  
kspace\_modify slab 3.0

#### Element Library (library.meam)

# library.meam  
'Mn' 'bcc' 8 25 54.94 5.0 2.5 1.0 1.0 1.0 2.72 3.0 0.90 1.0 3.0 2.0 -1.0 0.85 3  
'Fe' 'bcc' 8 26 55.847 5.07 2.94 1.0 1.0 1.0 2.864 4.29 0.89 1.0 3.94 4.12 -1.5 0.91 3  
'O' 'dim' 1 8 15.999 4.59 2.31 2.26 2.07 1.52 1.21 4.59 0.80 1.0 11.8 8.4 -6.2 2.6 3

Mn parameters: Cohesive energy (3.0 eV) from [Wang et al., PRB 2010], lattice const. (2.72 Å) from bcc-Mn.

#### Binary Parameters (mfo\_param.meam)

# mfo\_param.meam  
# Mn=1, Fe=2, O=3  
re(1,1)=2.70 # Mn-Mn (DFT: ~2.7 Å)  
re(2,2)=2.87 # Fe-Fe (FO-MEAM)  
re(3,3)=1.21 # O-O (FO-MEAM)  
delta(1,2)= -0.05 re(1,2)=2.60 alpha(1,2)=5.0 # Mn-Fe (L12 ref)  
lattce(1,3)='b1' delta(1,3)= -1.30 re(1,3)=2.10 alpha(1,3)=4.2 # Mn-O (MnO rock-salt)  
lattce(2,3)='b1' delta(2,3)= -1.365 re(2,3)=2.1475 alpha(2,3)=4.0 # Fe-O (FO-MEAM)  
rho0(1)=0.85 rho0(2)=0.91 rho0(3)=2.6  
emb\_lin\_neg=1  
bkgd\_dyn=1

#### LAMMPS Script (mfo\_meam.in)

# MEAM for MnFe2O4 Static Minimization  
pair\_style meam/c  
pair\_coeff \* \* library.meam Mn Fe O mfo\_param.meam Mn Fe O  
min\_style cg  
min\_modify dmax 0.001  
minimize 1e-25 1e-25 10000 10000

#### Nanostructure-Specific Additions

#### Surface Hydroxylation (3, 5, and 10 nm Sphere)

# After sphere cutoff in VESTA  
group surface id <surface\_Mn/Fe\_ids>  
set group surface type 4 # Assign new type for surface O  
pair\_style hybrid/overlay buck/coul/long 12.0 meam/c  
pair\_coeff 1 1\*3 meam/c library.meam Mn Fe O mfo\_param.meam Mn Fe O  
pair\_coeff 4 5 buck 450.0 1.0 0.0 # O(surf)-H (harmonic)  
bond\_style harmonic  
bond\_coeff 1 450.0 0.96 # O-H bond (k=450 kcal/mol·Å², r0=0.96 Å)  
create\_bonds single surface 4 5 1.0 # Connect surface O (type4) to H (type5)