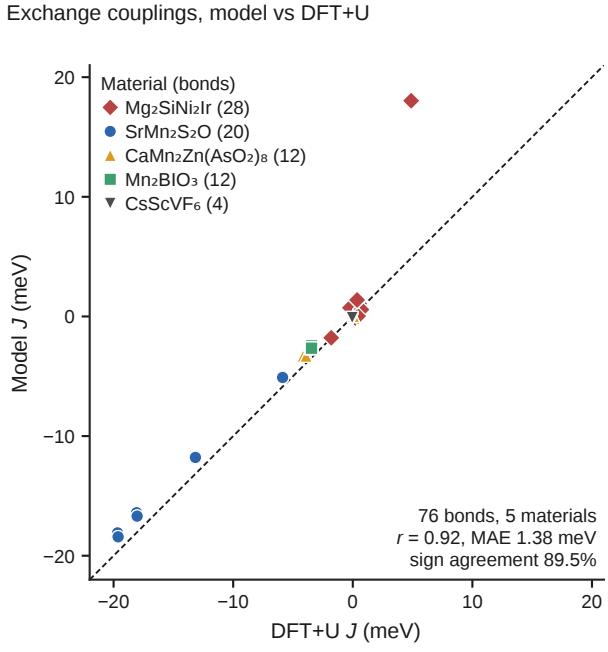

Exchange couplings, model vs DFT+U
Material (bonds)
Mg2SiNi2Ir (28)
SrMn2S2O (20)
CaMn2Zn(AsO2)8 (12)
Mn2BIO3 (12)
CsScVF6 (4)
76 bonds, 5 materials
r = 0.92, MAE 1.38 meV
sign agreement 89.5%
Model J (meV)
DFT+U J (meV)
20
10
0
−10
−20
−20
−10
0
10
20