

Foundation Models for Metallurgy?

Supplementary 1: Extra Figures for Main Potentials

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February 21, 2025

1 Bulk Property Tests

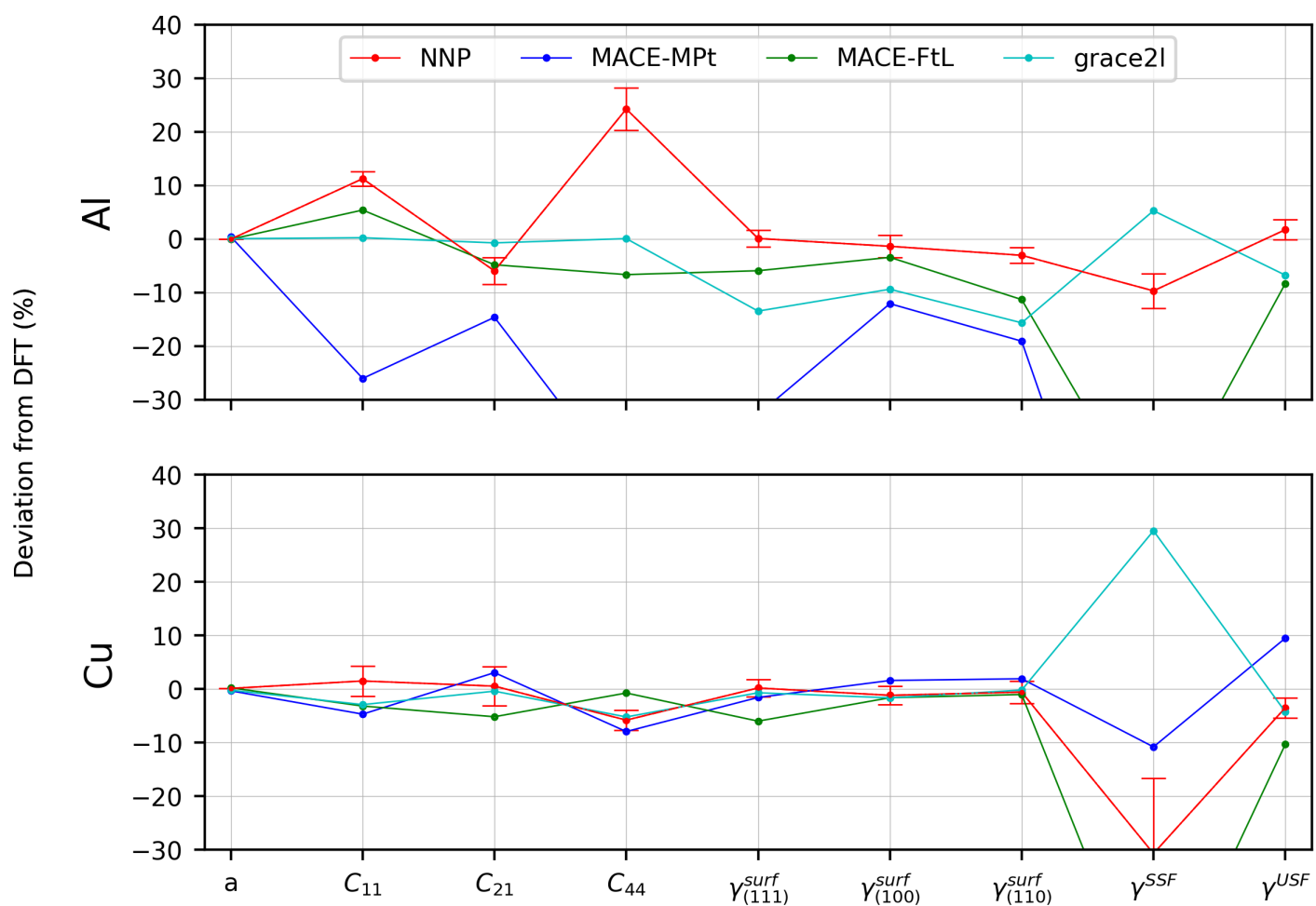


Figure S1-1: Plot of deviation from DFT (%) for key properties for Al and Cu

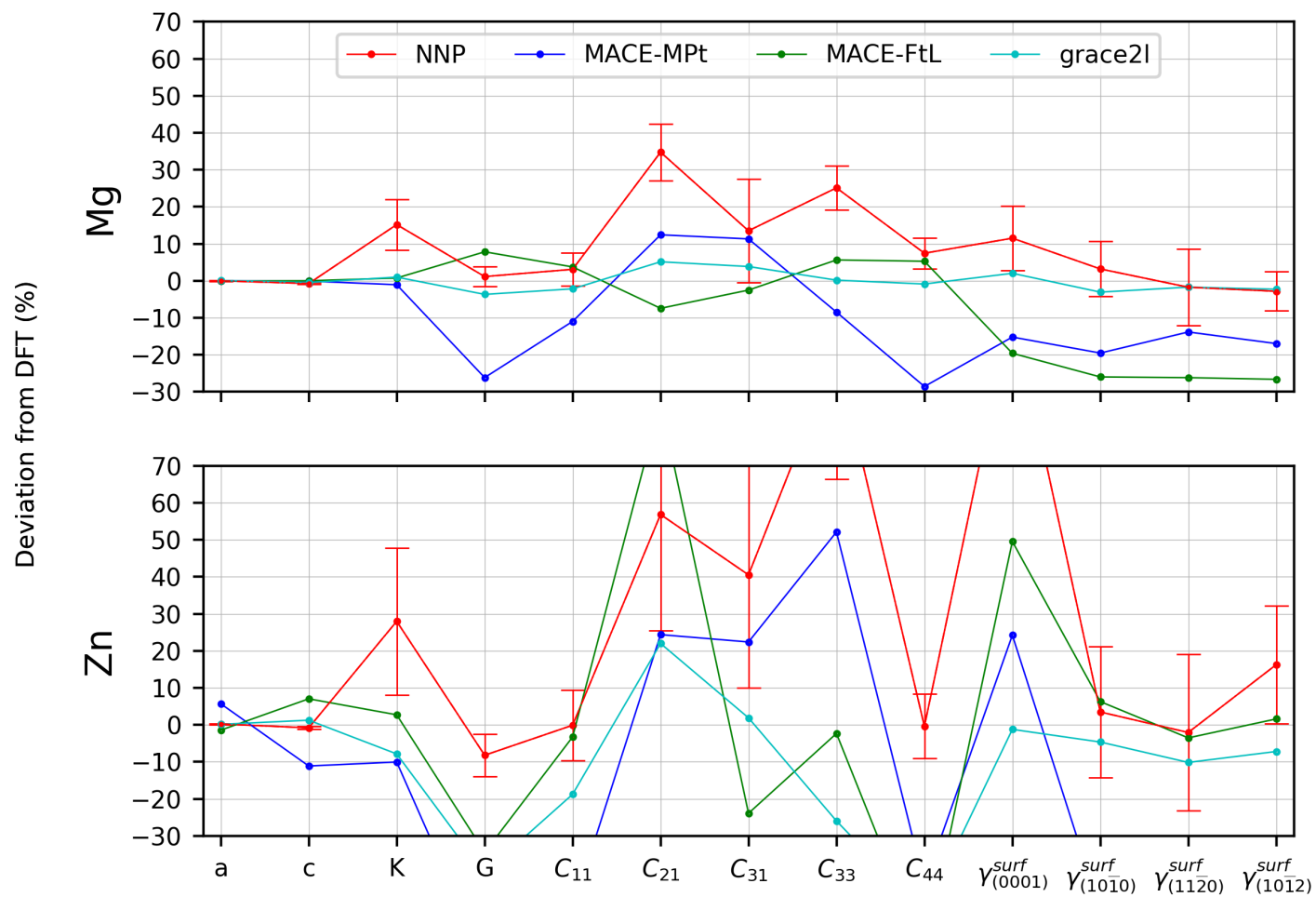


Figure S1-2: Plot of deviation from DFT (%) for key properties for Mg and Zn

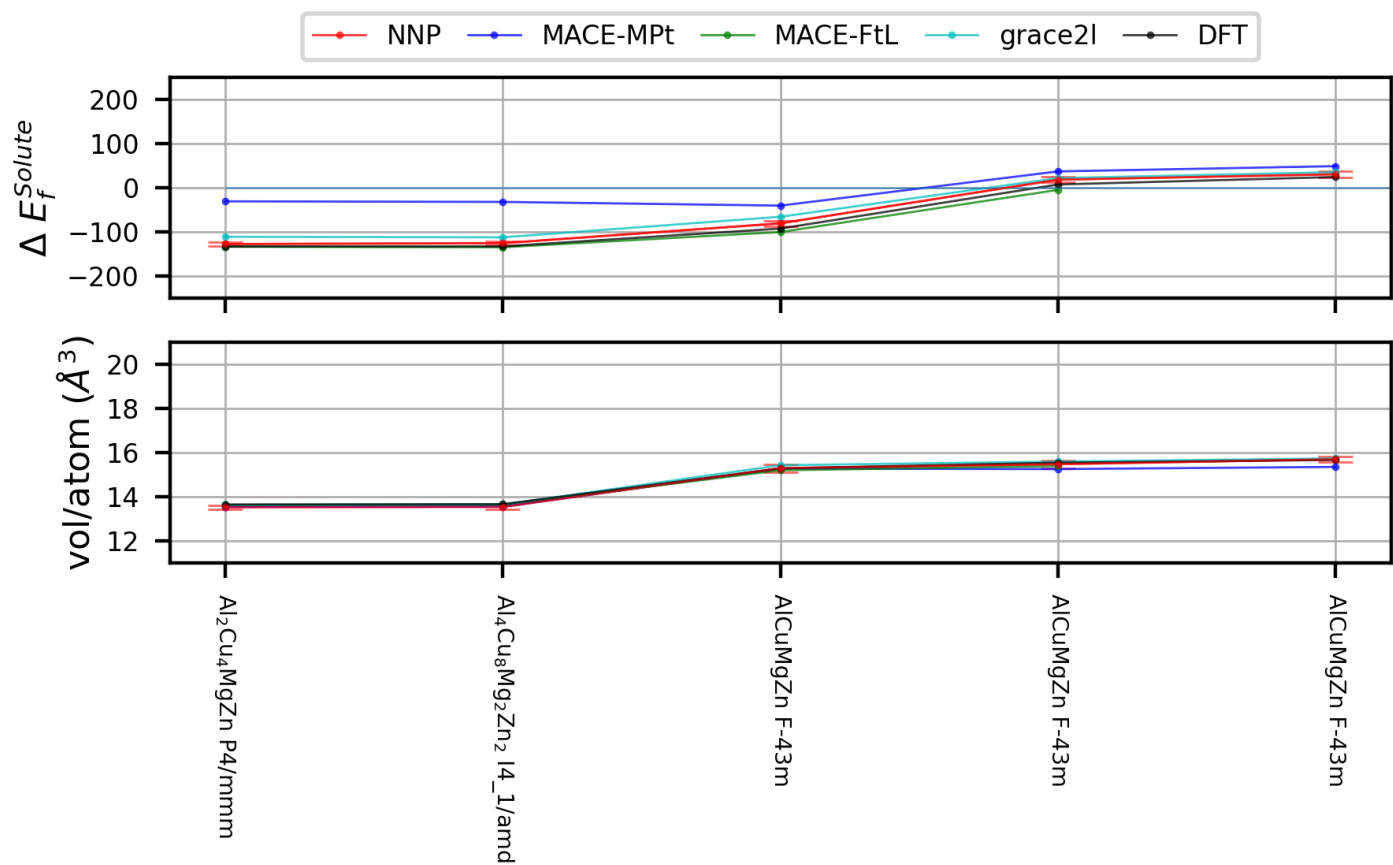


Figure S1-3: Plot of deviation from DFT (%) for key properties for Al Zn Cu Mg

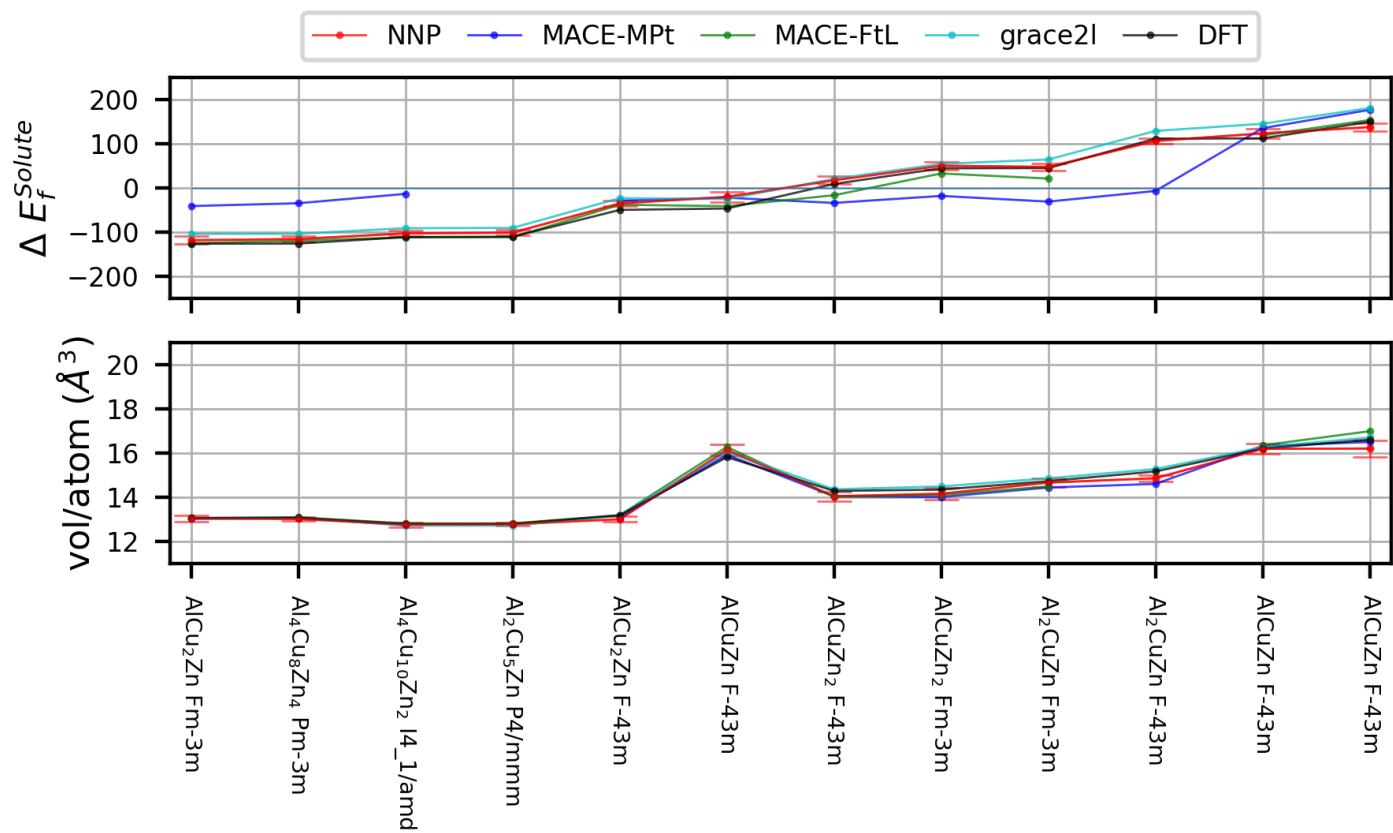


Figure S1-4: Plot of deviation from DFT (%) for key properties for Al Cu Zn

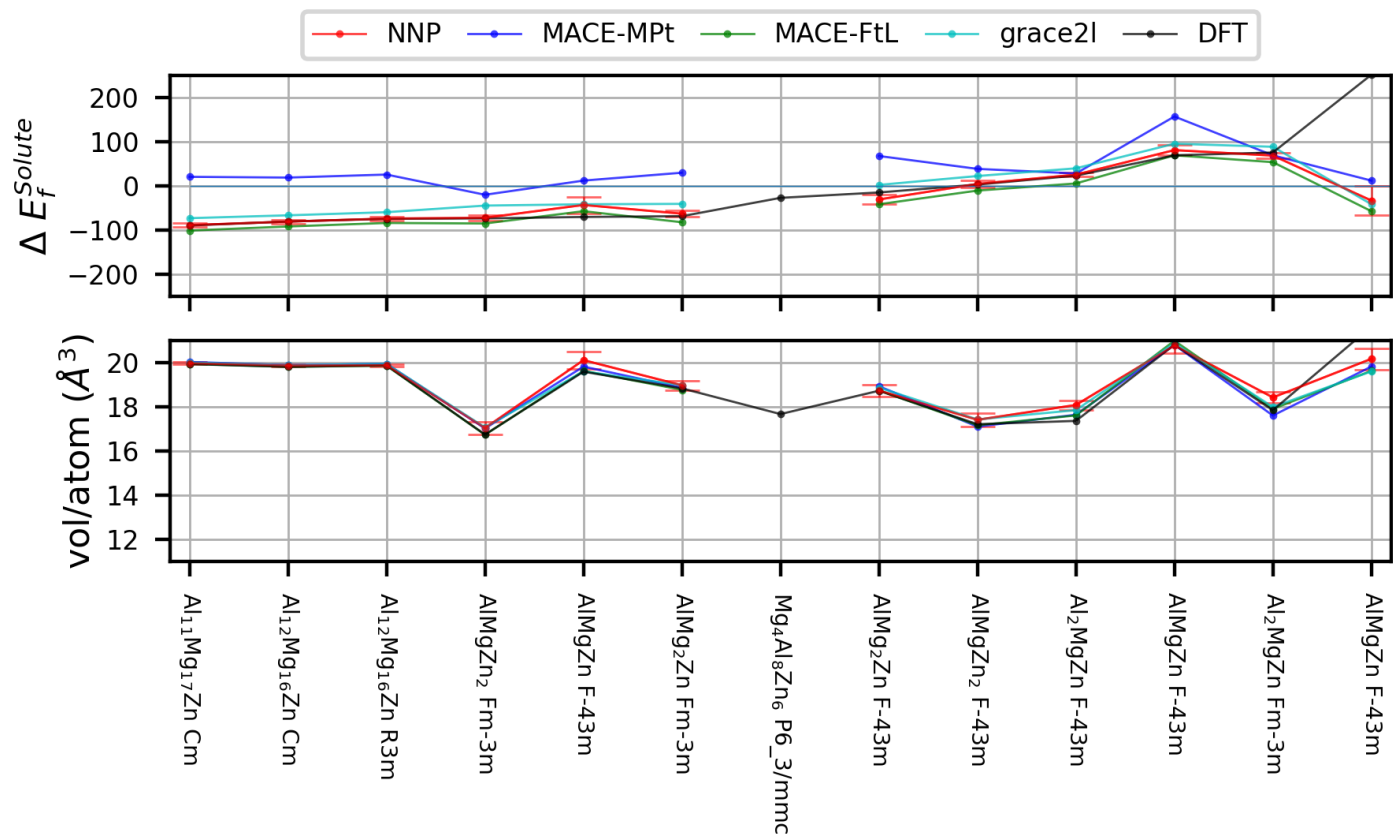
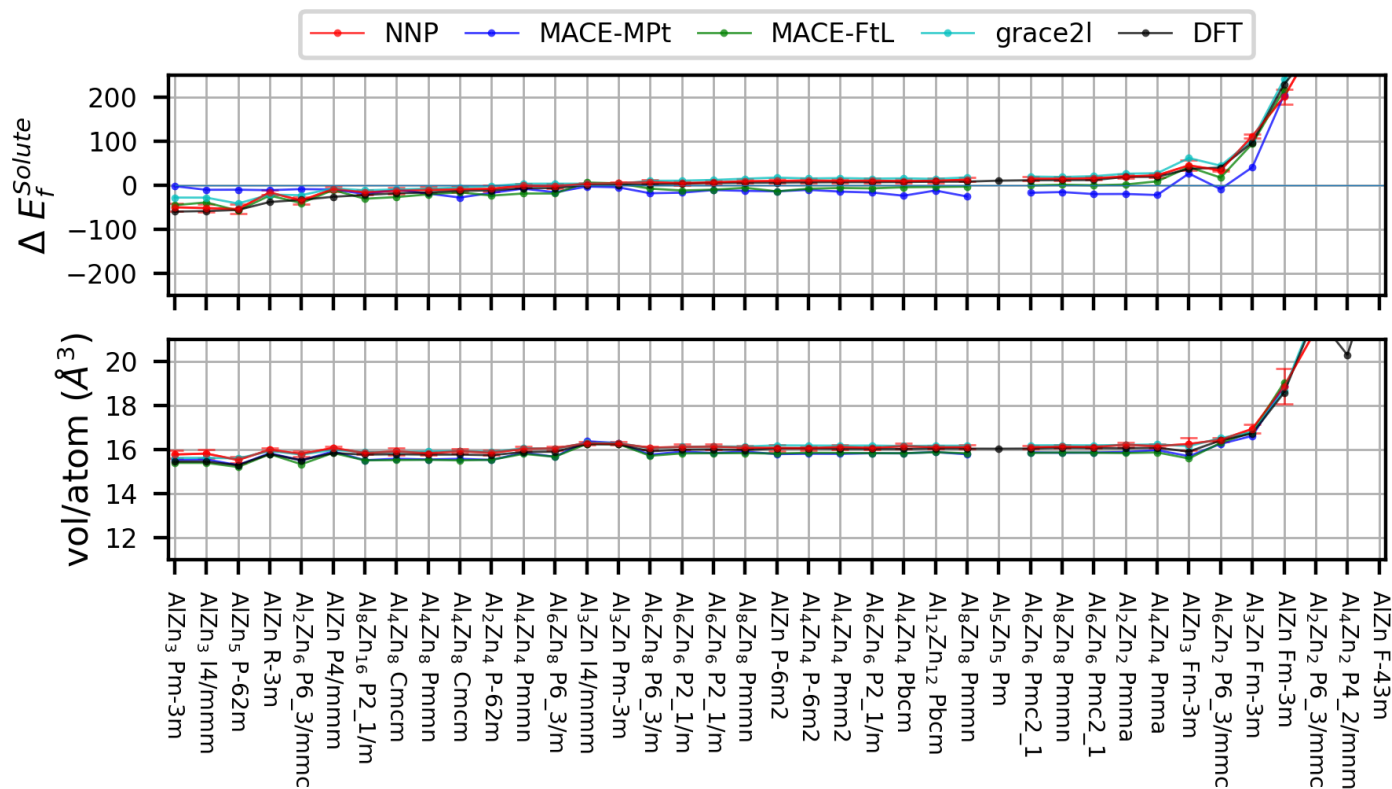
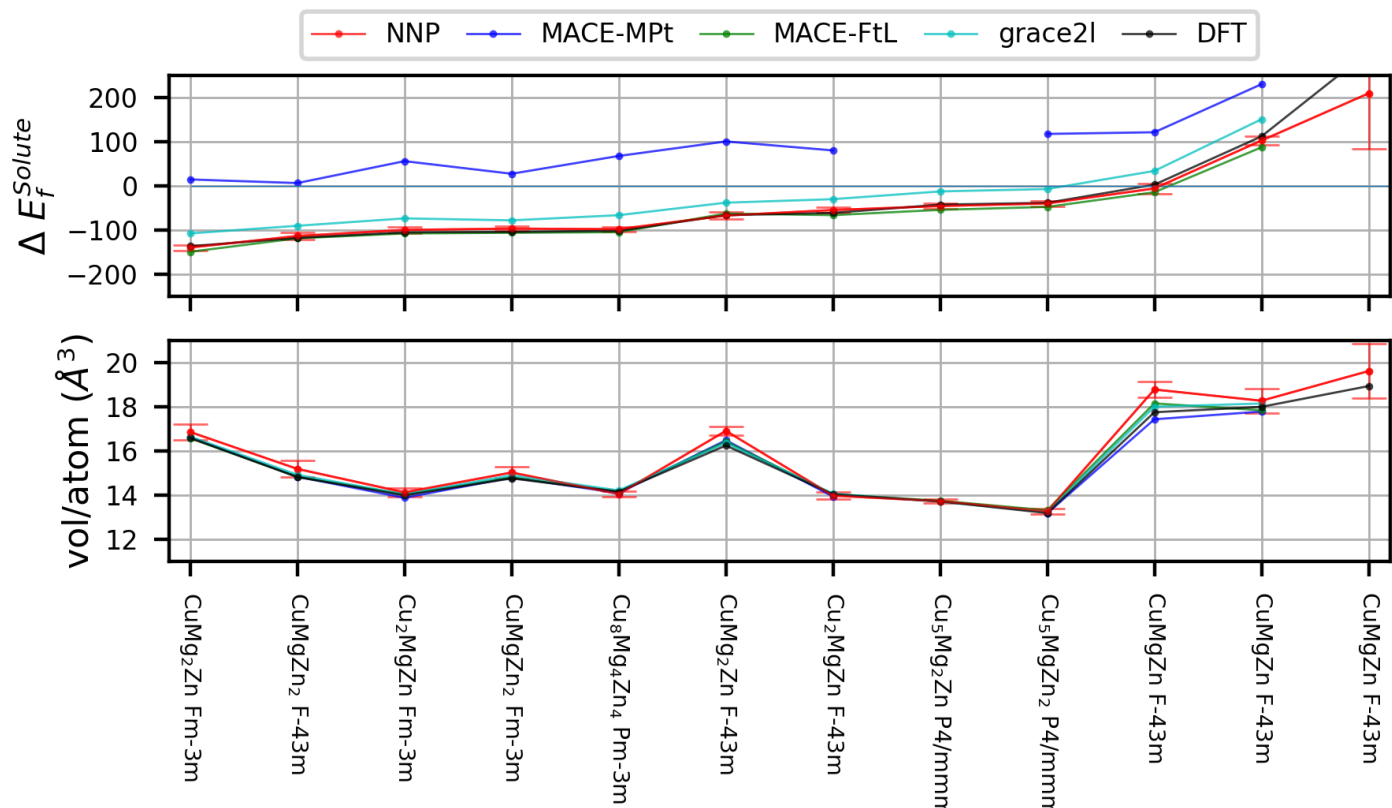
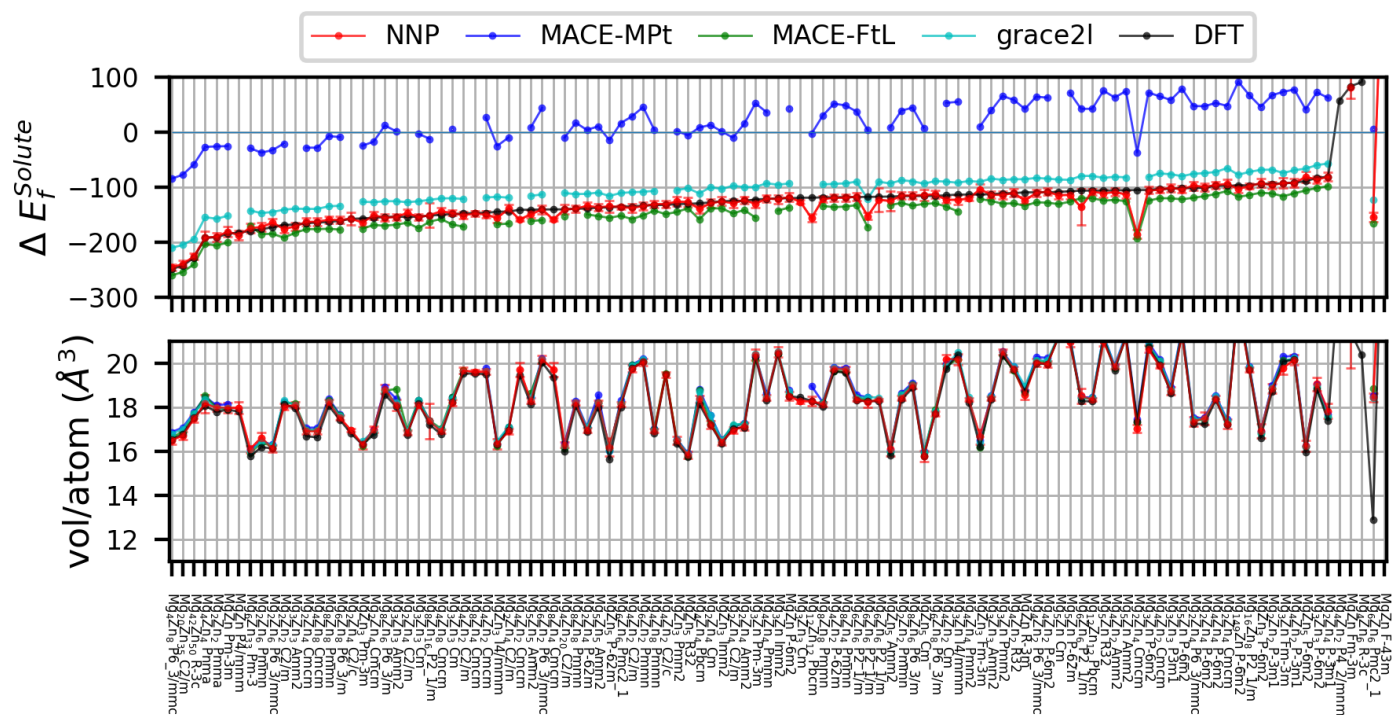
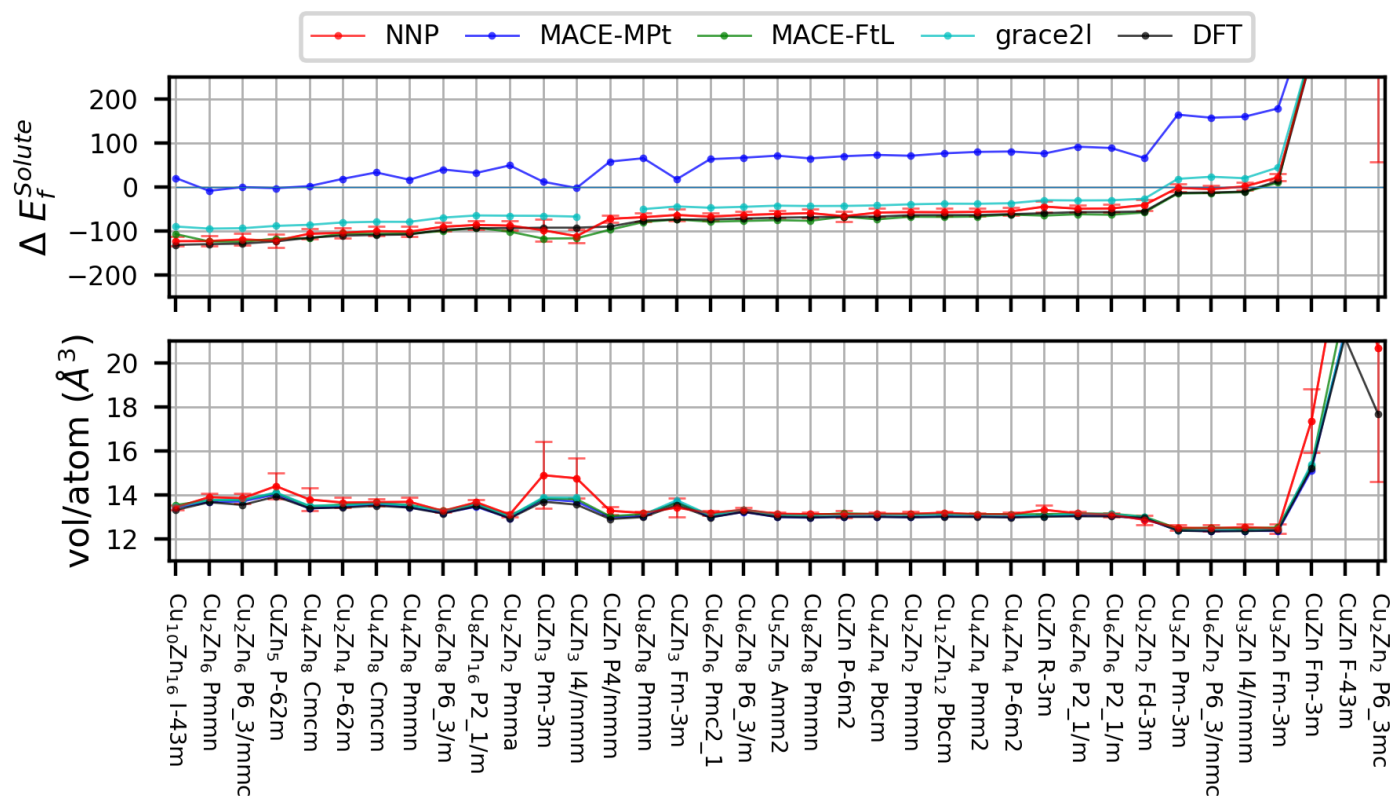


Figure S1-5: Plot of deviation from DFT (%) for key properties for Al Mg Zn





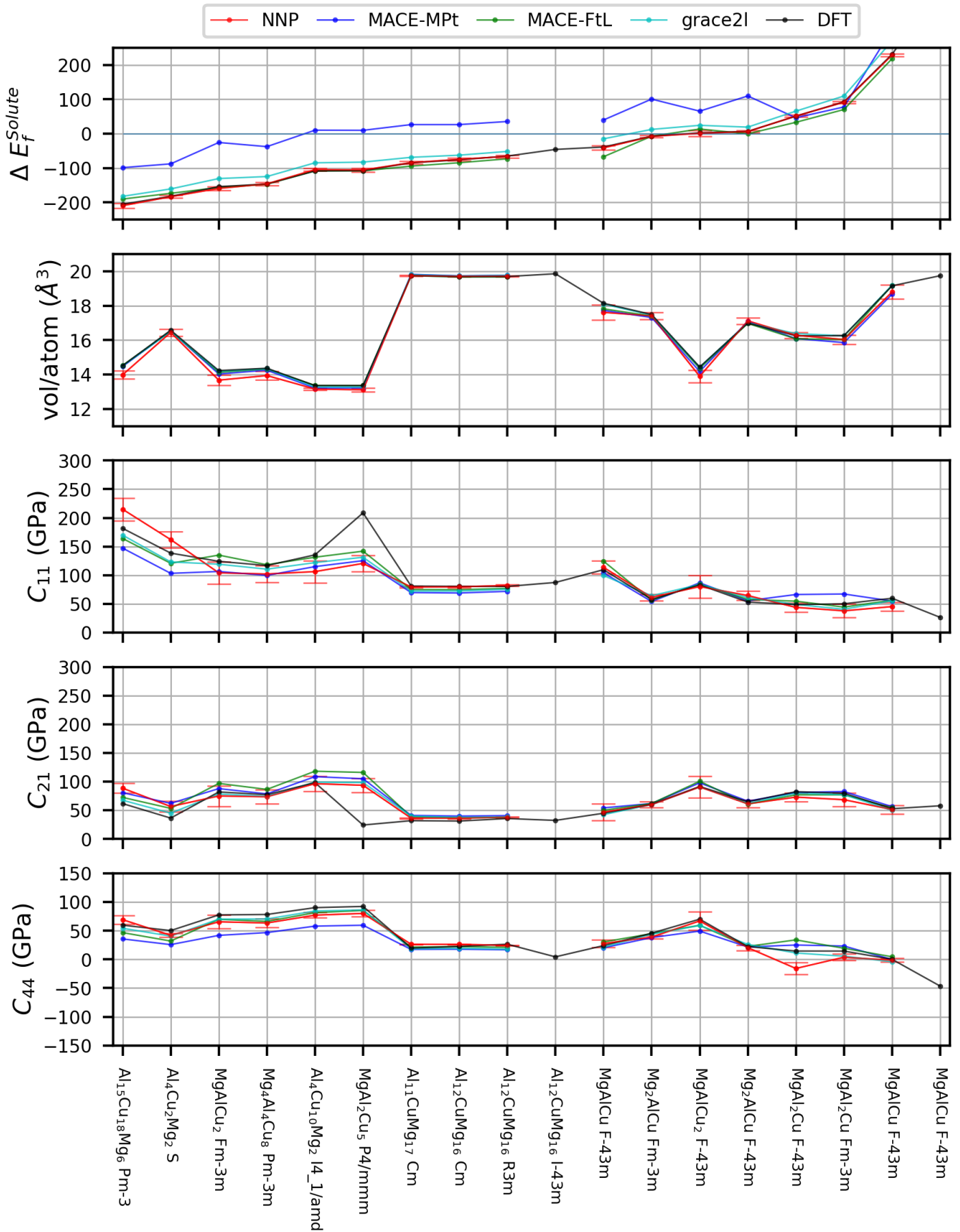


Figure S1-10: Plot of formation energy (meV), atomic volume ($\text{\AA}^3$) C_{11} , C_{21} and C_{44} (GPa) for all AlCuMg structures in OQMD.

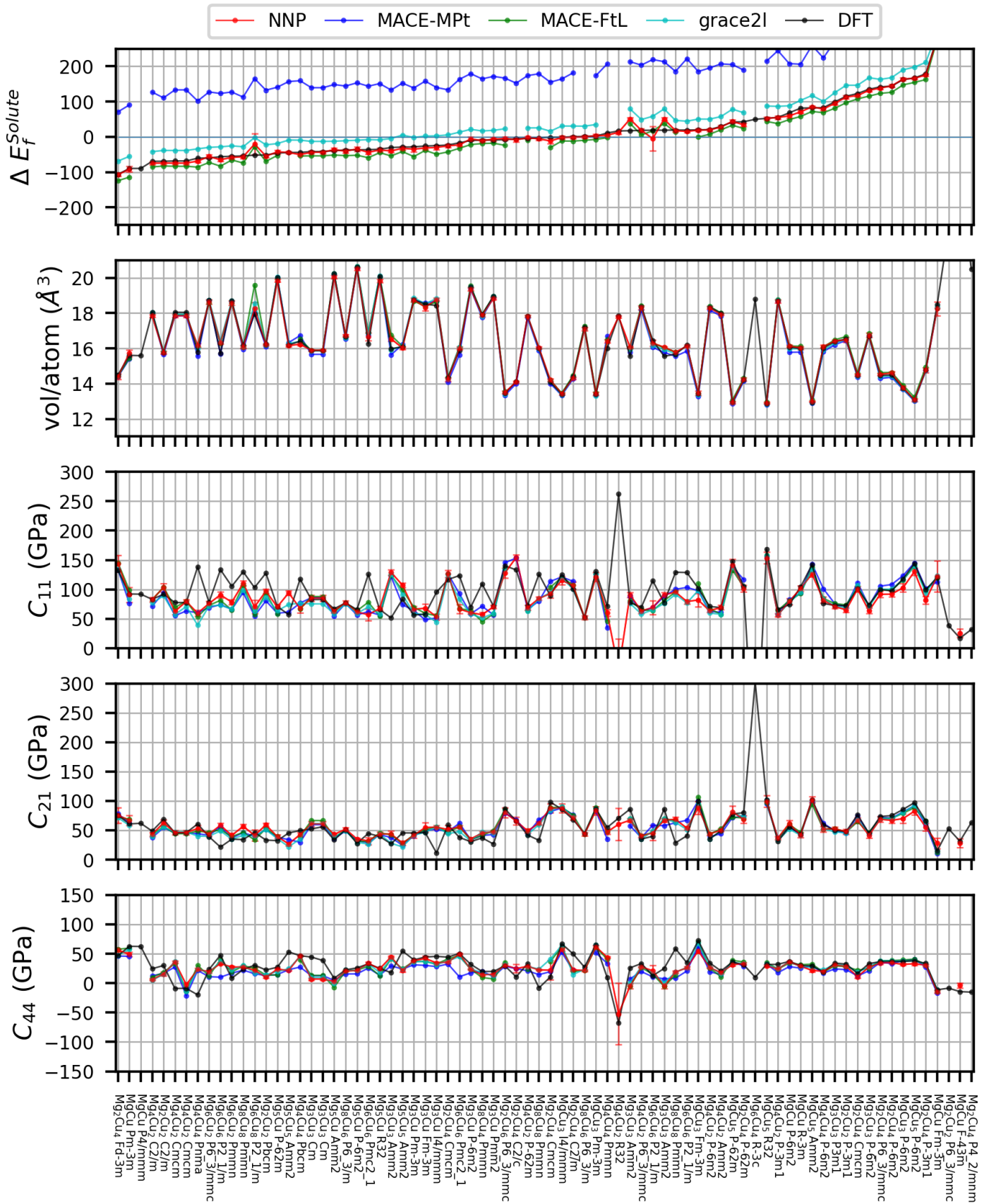


Figure S1-12: Plot of formation energy (meV), atomic volume ($\text{\AA}^3$) C_{11} , C_{21} and C_{44} (GPa) for all CuMg structures in OQMD.

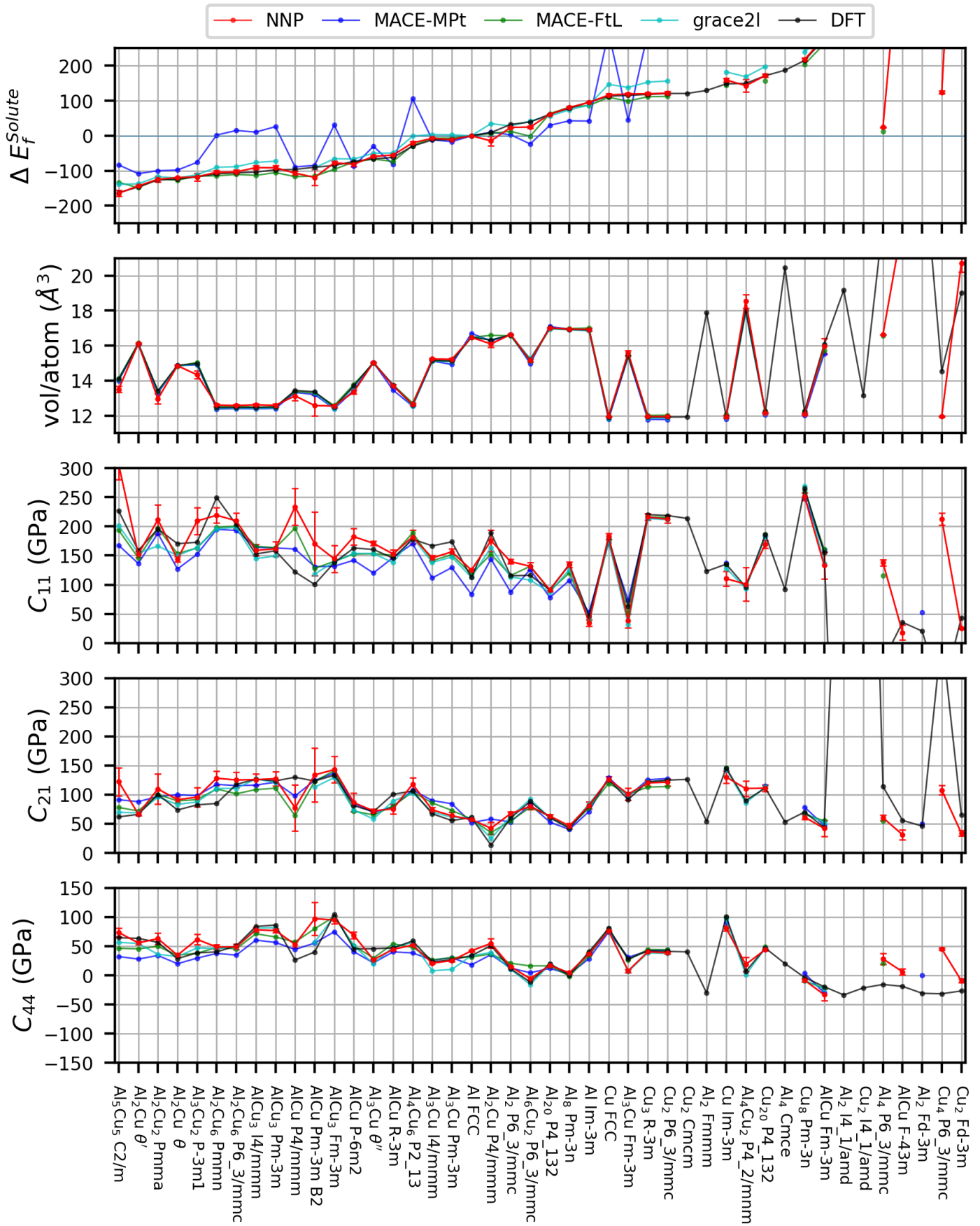


Figure S1-13: Plot of formation energy (meV), atomic volume ($\text{\AA}^3$) C_{11} , C_{21} and C_{44} (GPa) for all AlCu structures in OQMD.

2 Solute Tests

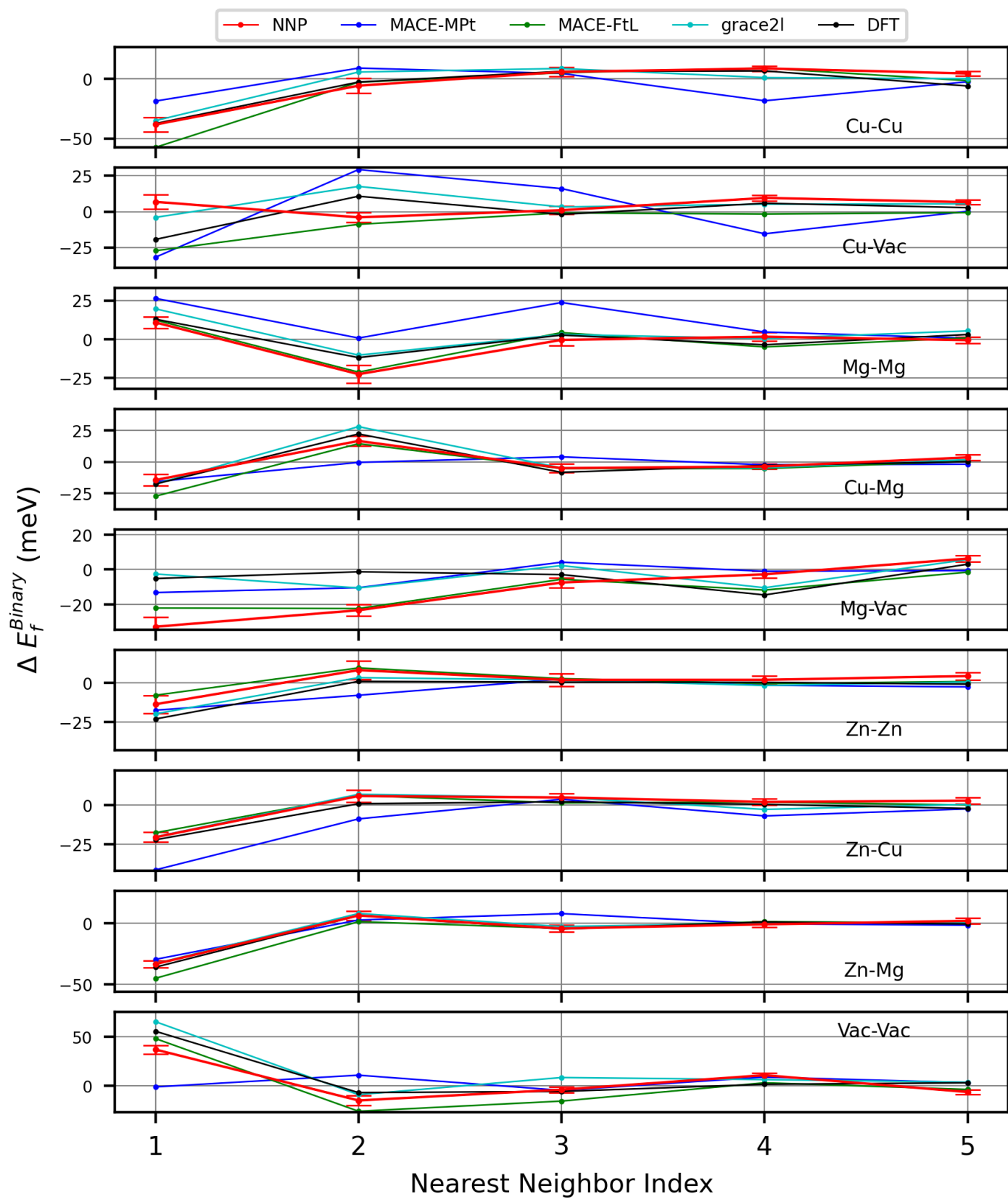


Figure S1-14: Sol-Sol binding energy (in meV) in Al matrix

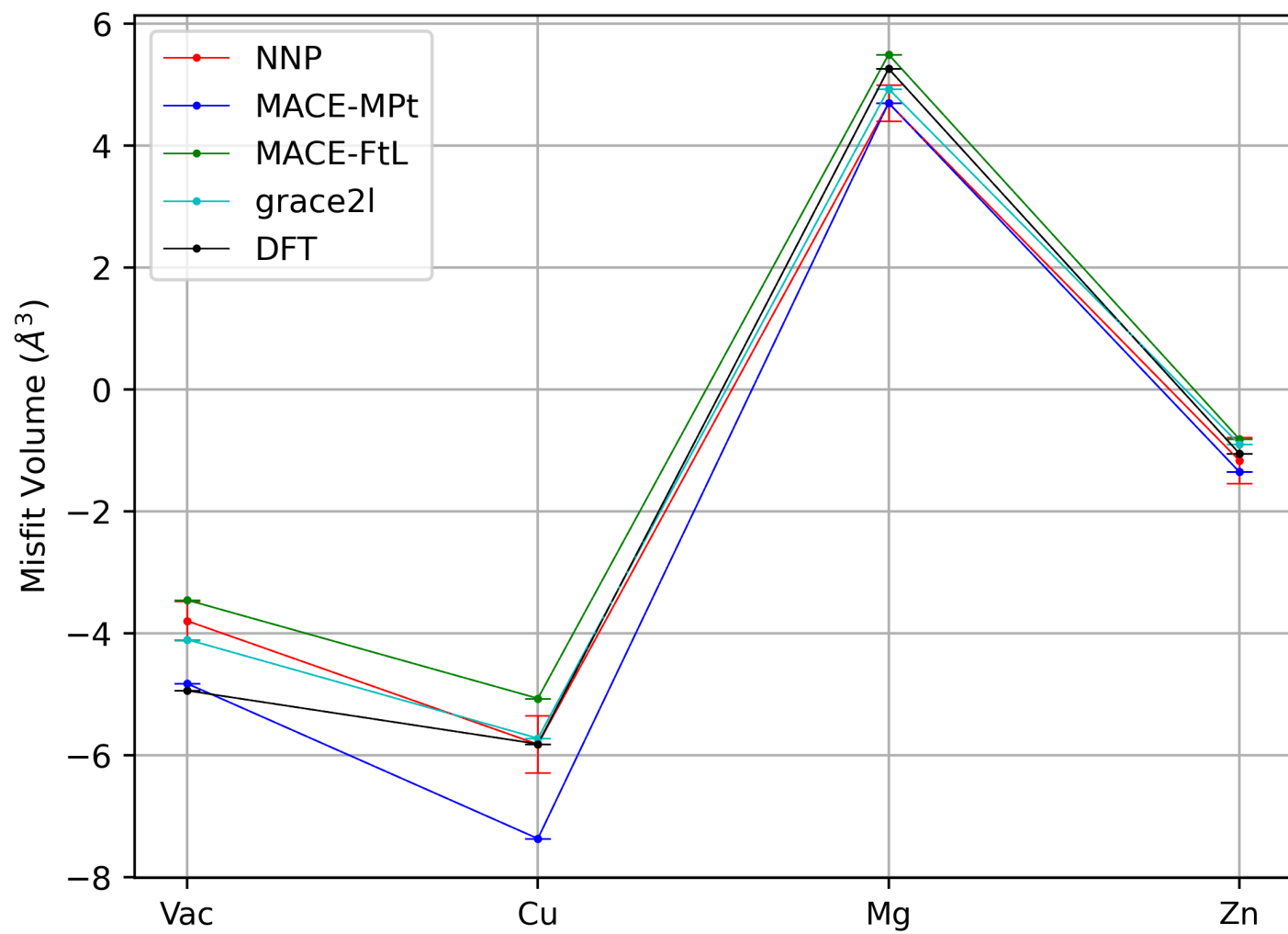


Figure S1-15: Misfit volumes of Vac, Mg, and Cu in Al matrix.

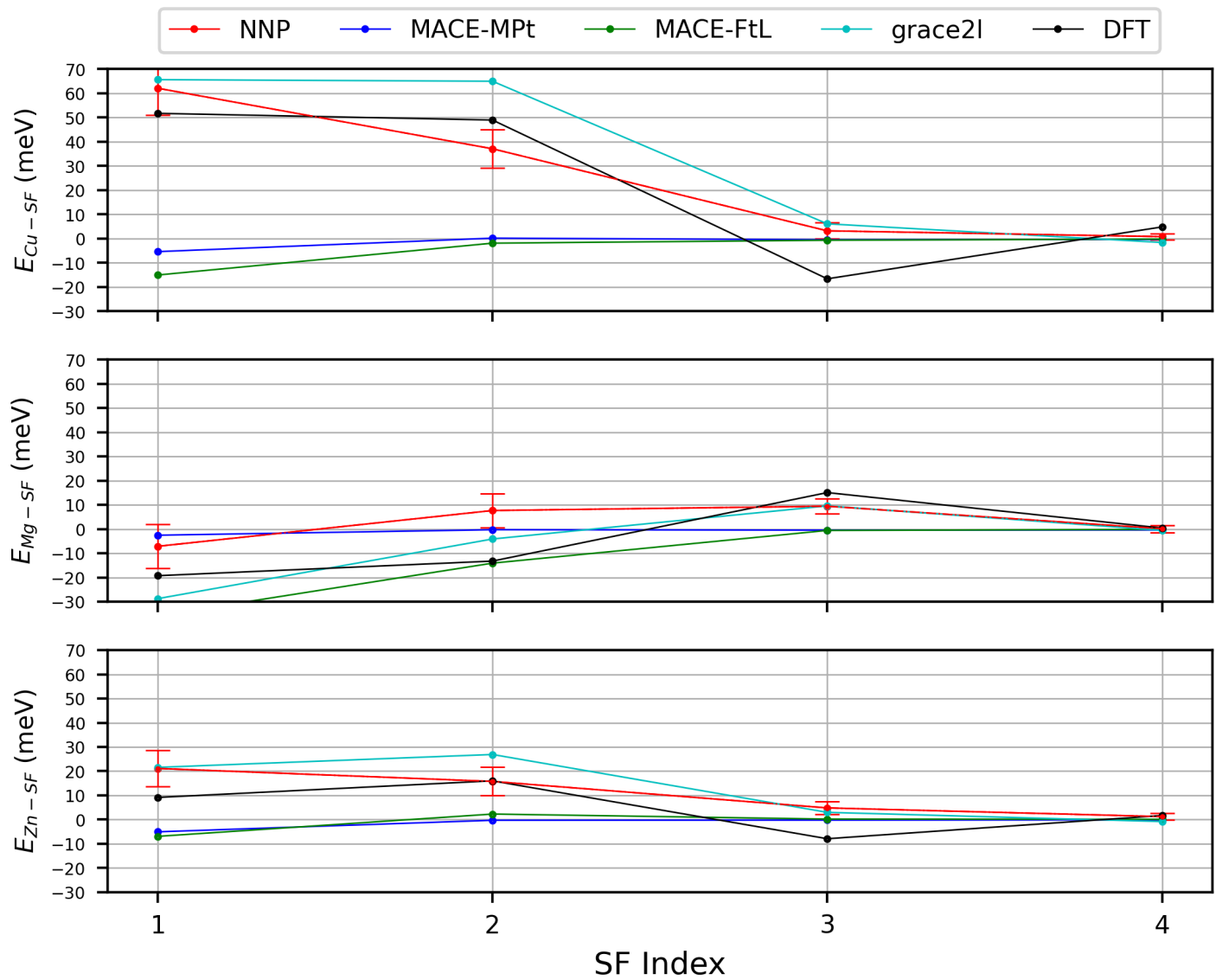


Figure S1-16: Solute-stacking fault interaction energies for Mg & Cu in Al matrix

3 Cluster Tests

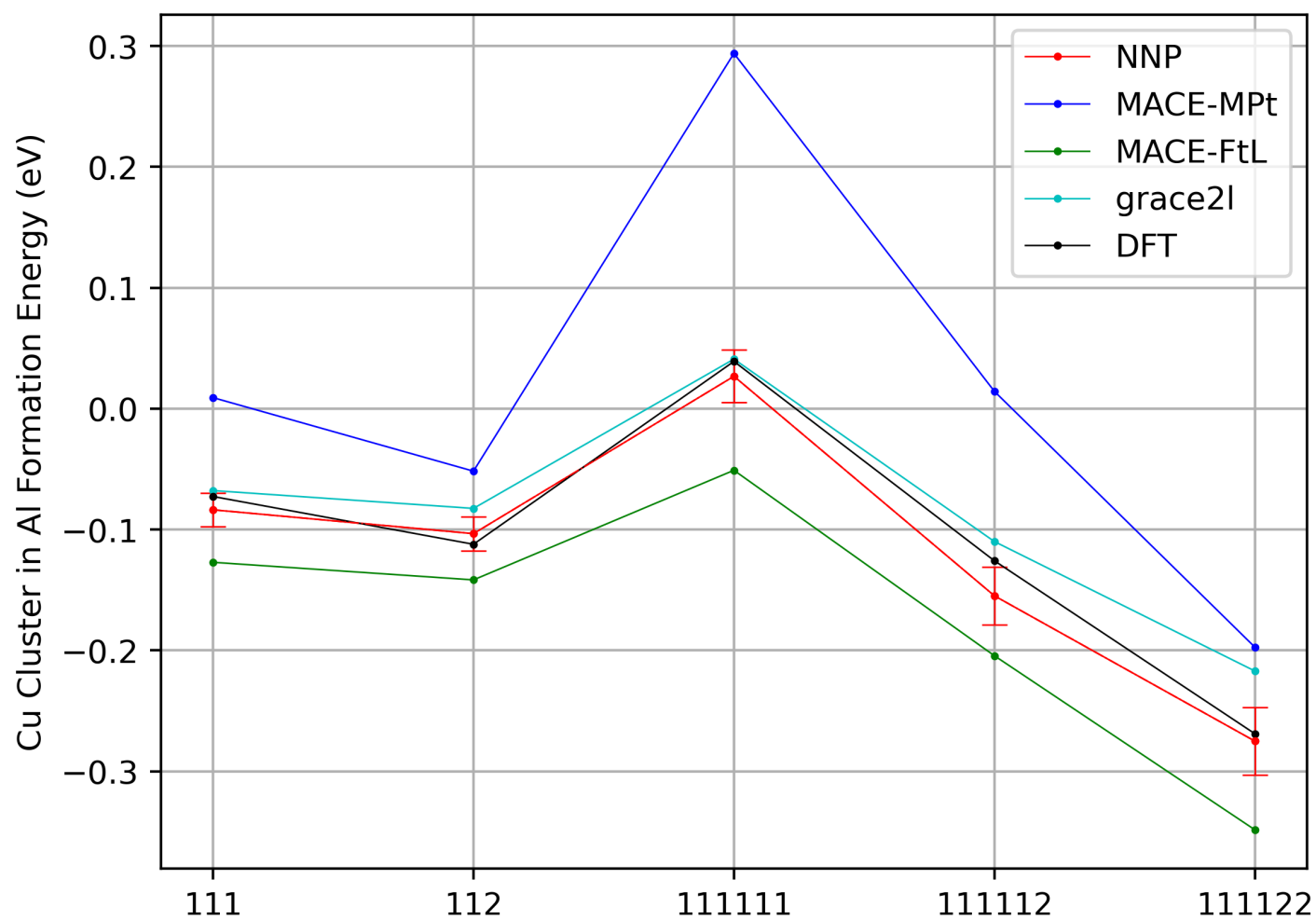


Figure S1-17: Cu cluster energies (eV) in Al matrix

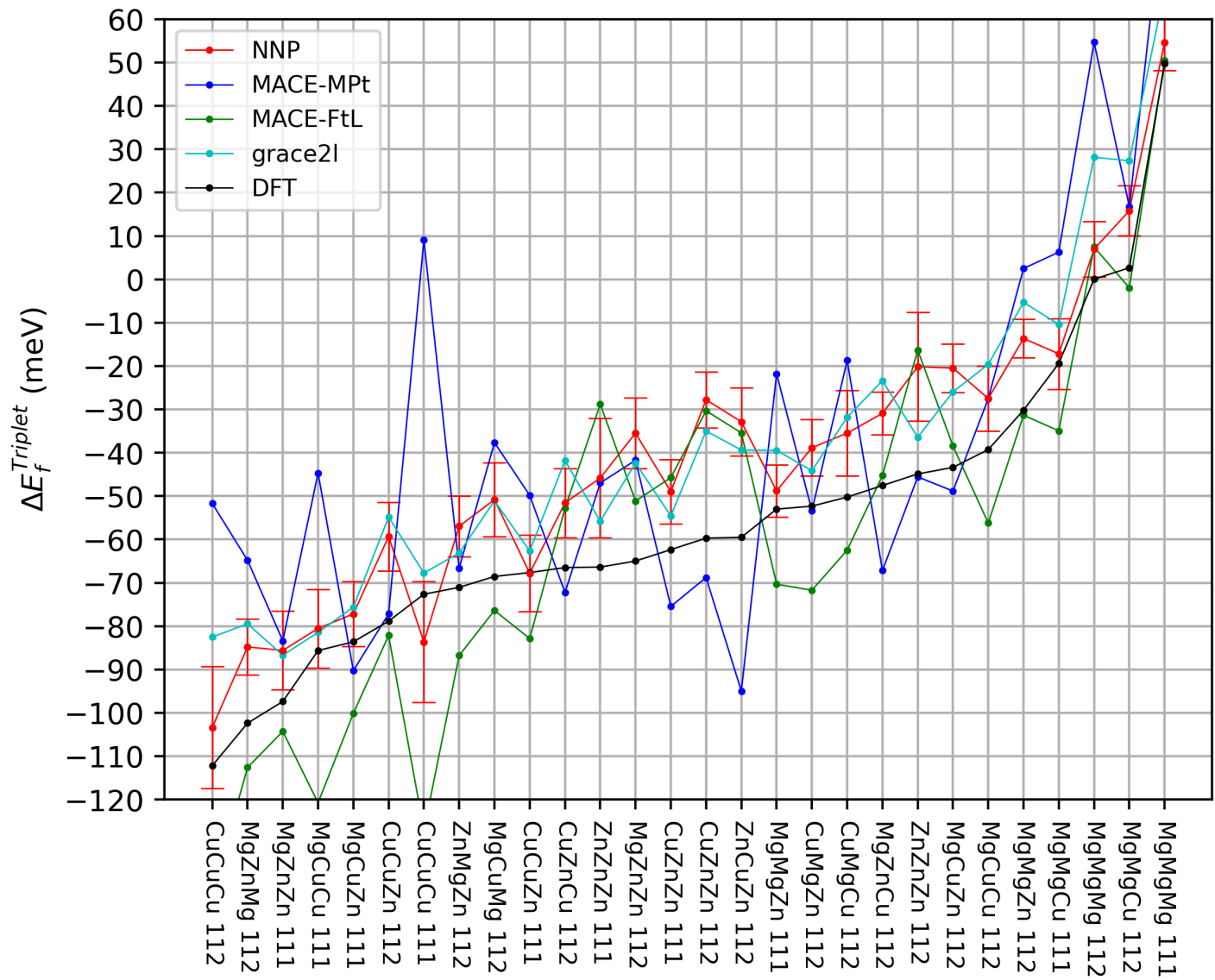


Figure S1-18: Triplet energies (meV) in Al matrix

4 GSF Tests

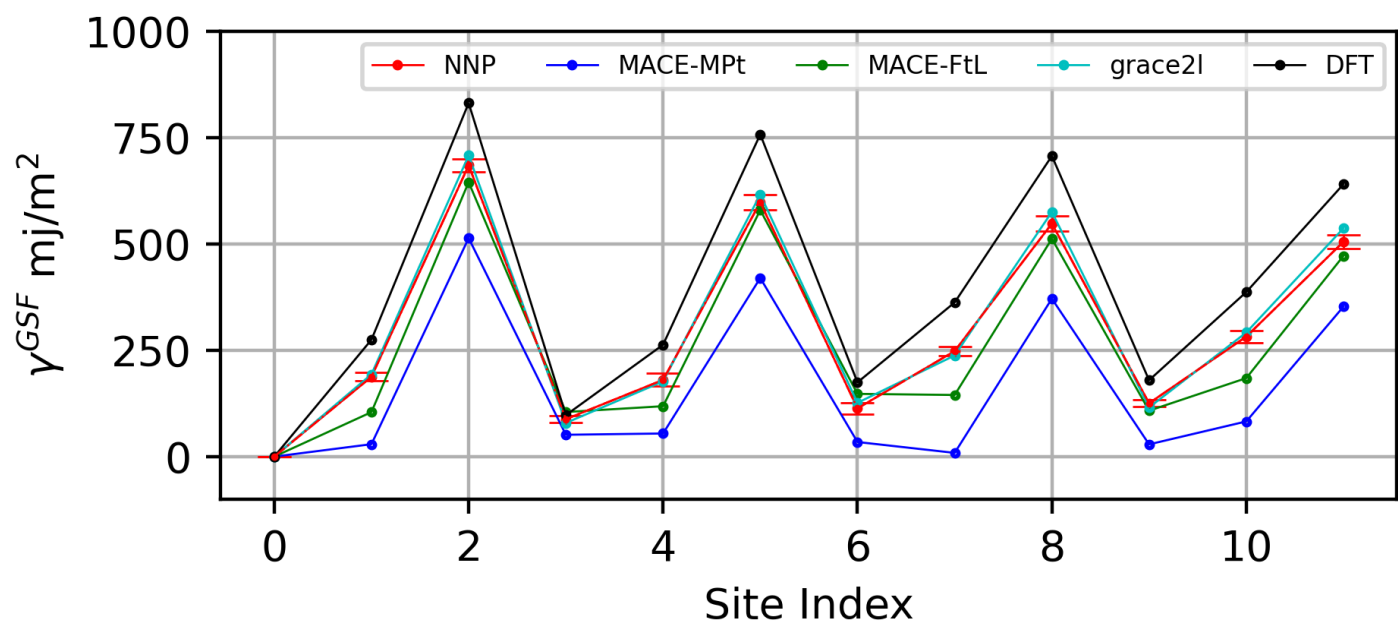


Figure S1-19: GSF energy for key sites on the 111 surface of θ'' .

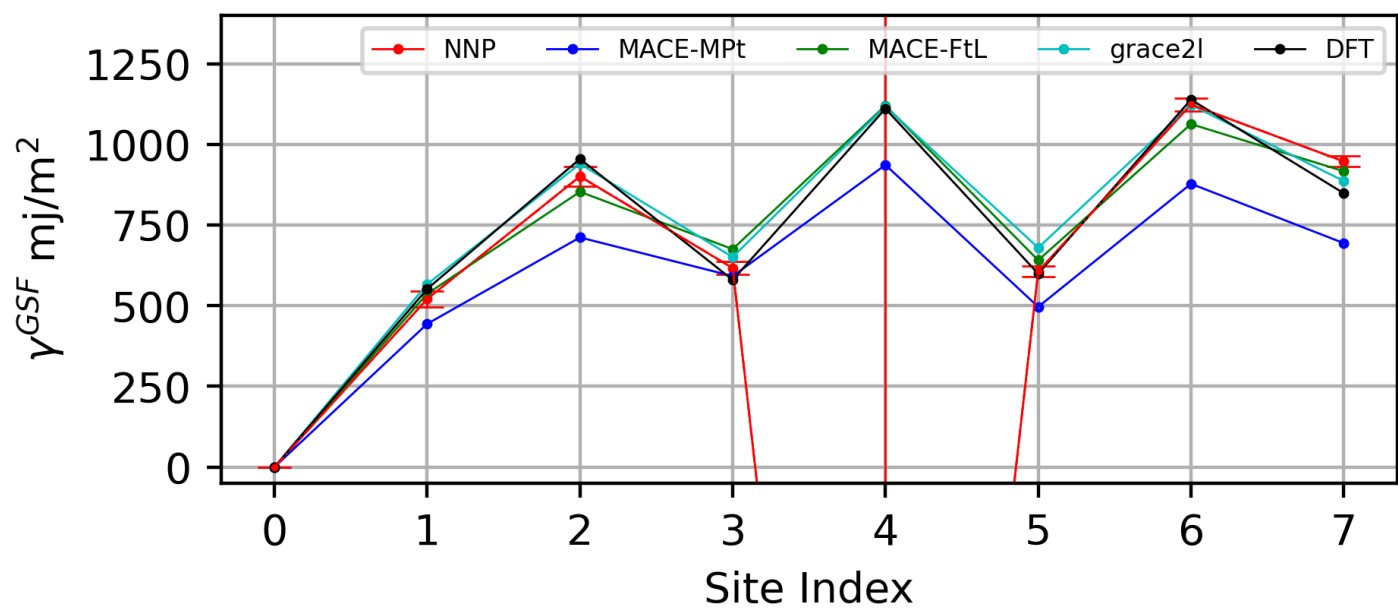


Figure S1-20: GSF energy for key sites on the 0-11 surface of θ .

5 Antisite Tests

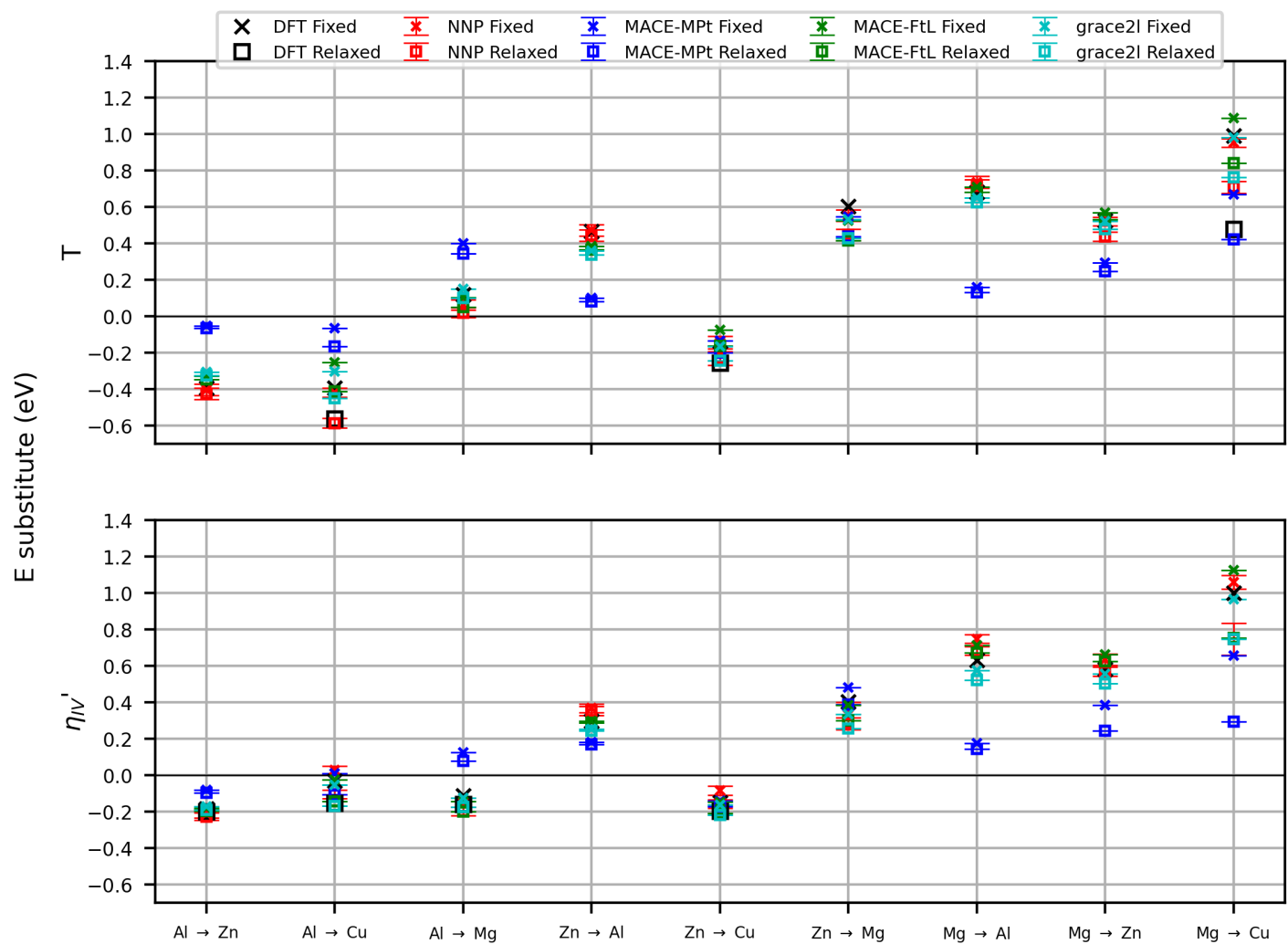


Figure S1-21: Antisite energies (EtaP IV)

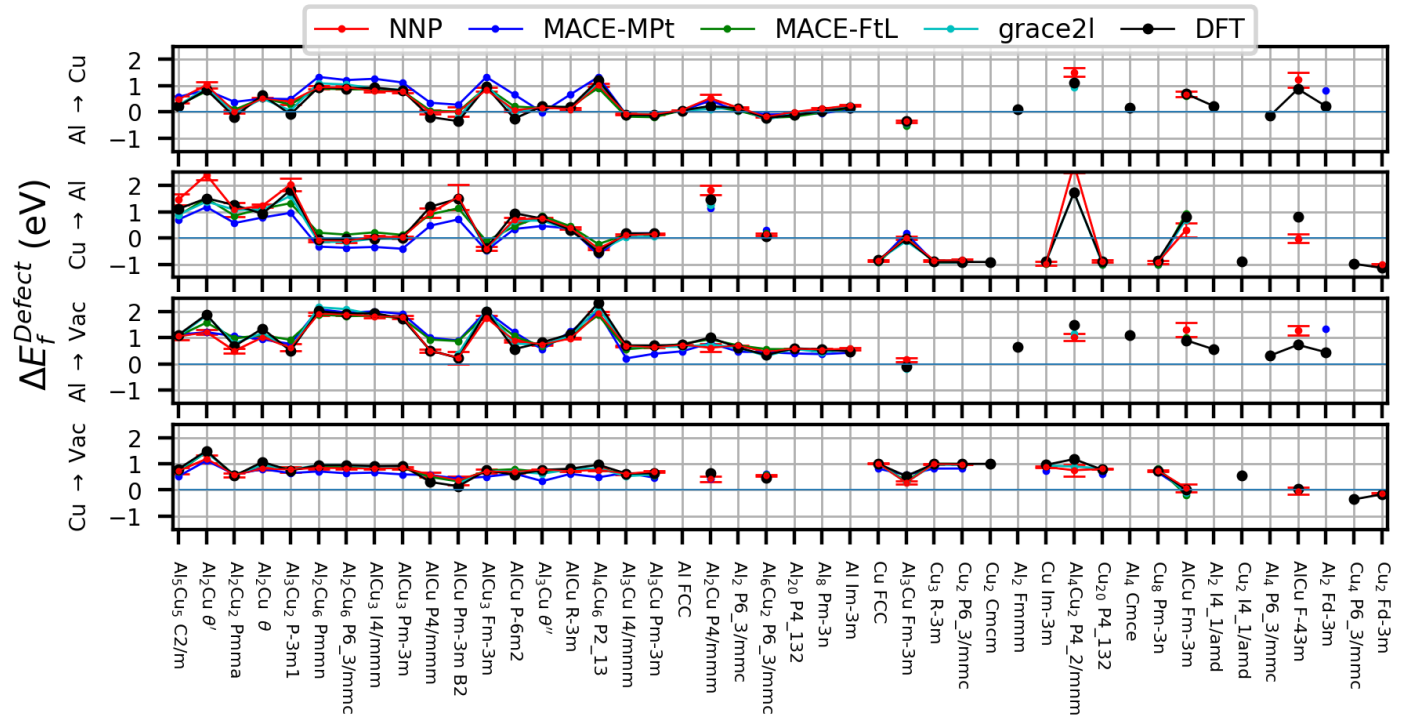


Figure S1-22: Antisite energies for Al-Cu compounds

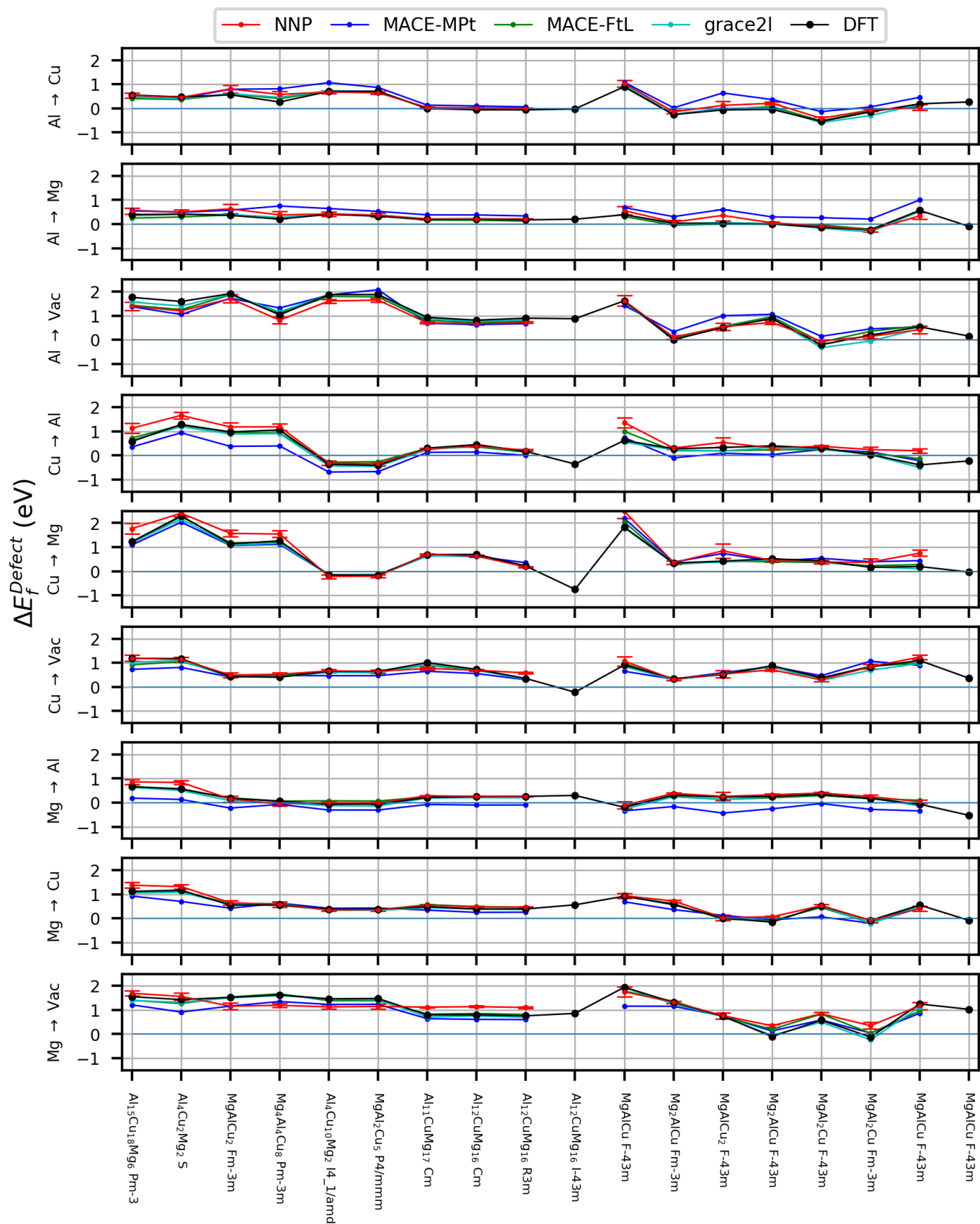


Figure S1-23: Antisite energies for Al-Cu-Mg compounds