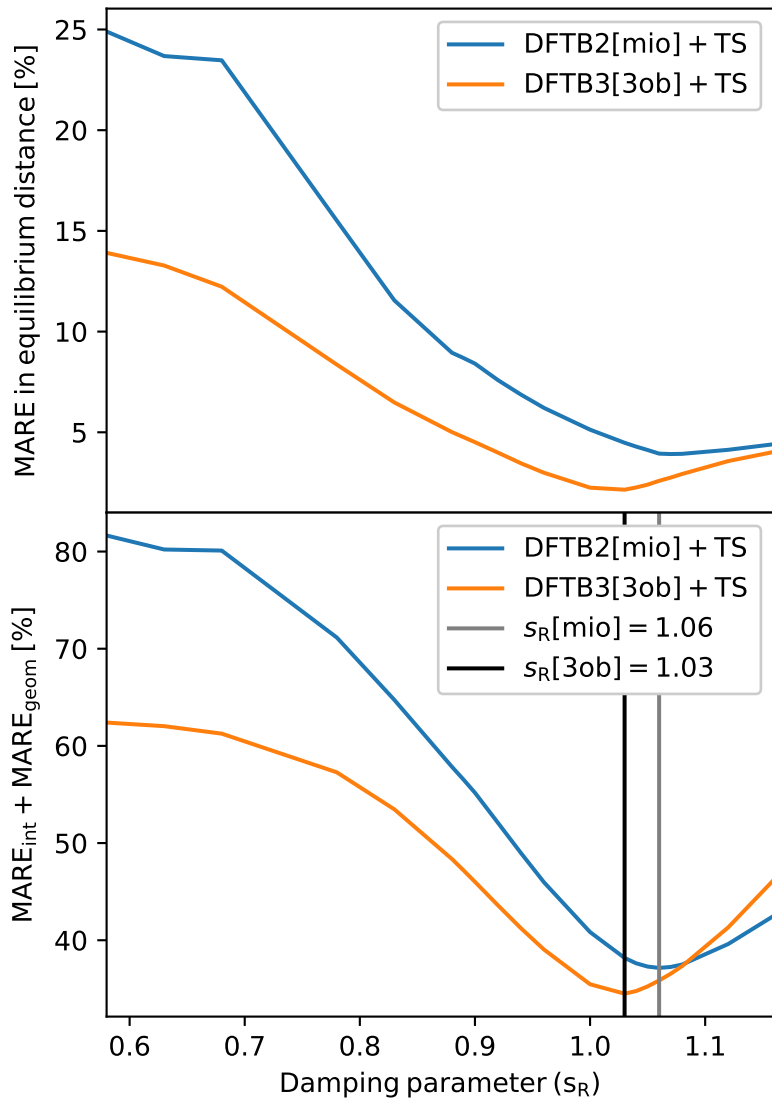


Geometrical aspects S66x8



DFTB + TS interaction energies

