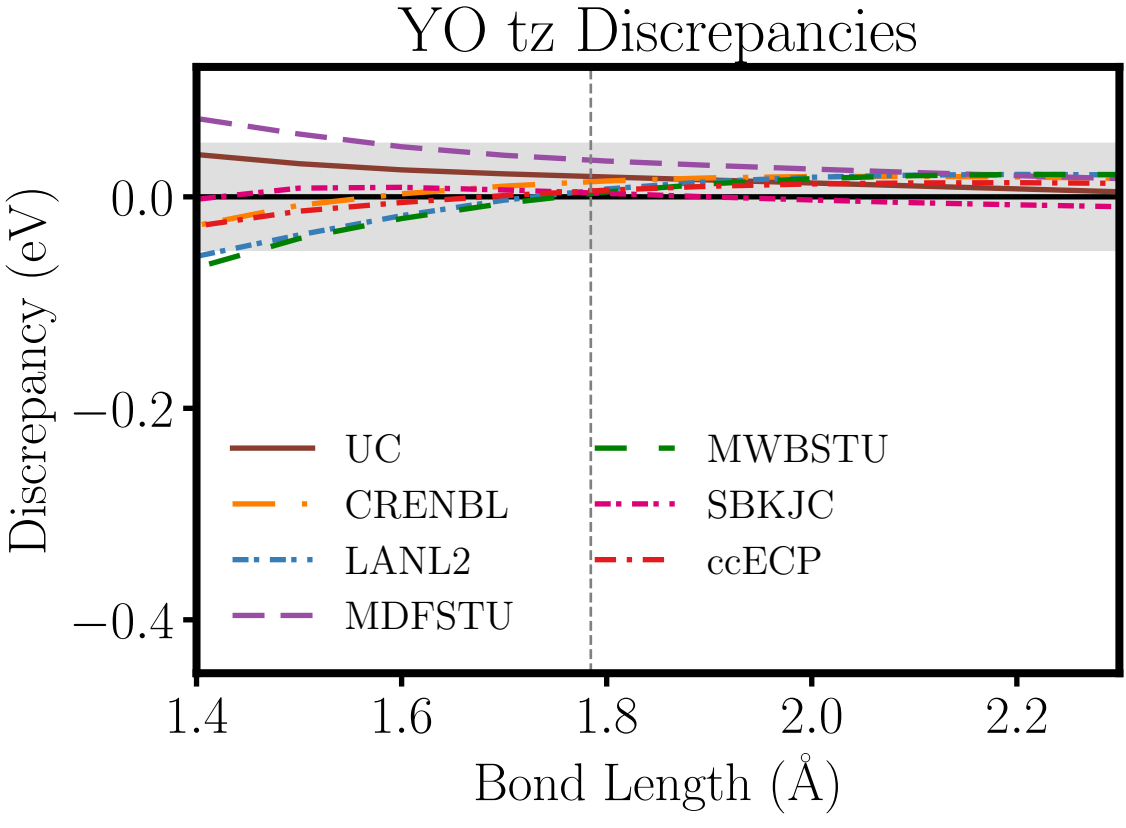
YO tz Discrepancies
Discrepancy (eV)
0.0
−0.2
−0.4
1.4
1.6
1.8
2.0
2.2
Bond Length (Å)
UC
CRENBL
LANL2
MDFSTU
MWBSTU
SBKJC
ccECP