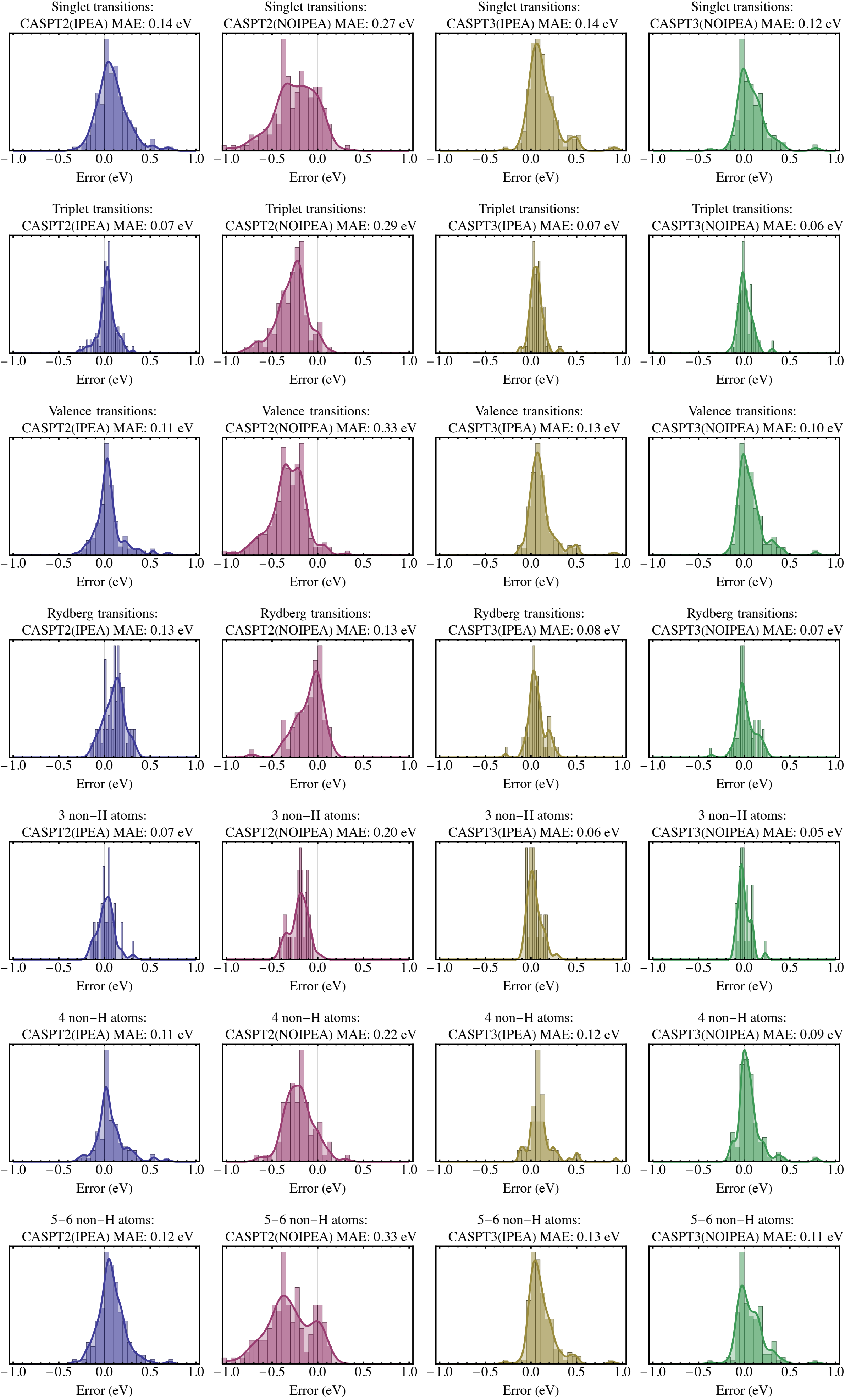
Singlet transitions:
CASPT2(IPEA) MAE: 0.14 eV
Singlet transitions:
CASPT2(NOIPEA) MAE: 0.27 eV
Singlet transitions:
CASPT3(IPEA) MAE: 0.14 eV
Singlet transitions:
CASPT3(NOIPEA) MAE: 0.12 eV
Triplet transitions:
CASPT2(IPEA) MAE: 0.07 eV
Triplet transitions:
CASPT2(NOIPEA) MAE: 0.29 eV
Triplet transitions:
CASPT3(IPEA) MAE: 0.07 eV
Triplet transitions:
CASPT3(NOIPEA) MAE: 0.06 eV
Valence transitions:
CASPT2(IPEA) MAE: 0.11 eV
Valence transitions:
CASPT2(NOIPEA) MAE: 0.33 eV
Valence transitions:
CASPT3(IPEA) MAE: 0.13 eV
Valence transitions:
CASPT3(NOIPEA) MAE: 0.10 eV
Rydberg transitions:
CASPT2(IPEA) MAE: 0.13 eV
Rydberg transitions:
CASPT2(NOIPEA) MAE: 0.13 eV
Rydberg transitions:
CASPT3(IPEA) MAE: 0.08 eV
Rydberg transitions:
CASPT3(NOIPEA) MAE: 0.07 eV
3 non−H atoms:
CASPT2(IPEA) MAE: 0.07 eV
3 non−H atoms:
CASPT2(NOIPEA) MAE: 0.20 eV
3 non−H atoms:
CASPT3(IPEA) MAE: 0.06 eV
3 non−H atoms:
CASPT3(NOIPEA) MAE: 0.05 eV
4 non−H atoms:
CASPT2(IPEA) MAE: 0.11 eV
4 non−H atoms:
CASPT2(NOIPEA) MAE: 0.22 eV
4 non−H atoms:
CASPT3(IPEA) MAE: 0.12 eV
4 non−H atoms:
CASPT3(NOIPEA) MAE: 0.09 eV
5−6 non−H atoms:
CASPT2(IPEA) MAE: 0.12 eV
5−6 non−H atoms:
CASPT2(NOIPEA) MAE: 0.33 eV
5−6 non−H atoms:
CASPT3(IPEA) MAE: 0.13 eV
5−6 non−H atoms:
CASPT3(NOIPEA) MAE: 0.11 eV
−1.0 −0.5 0.0 0.5 1.0
Error (eV)