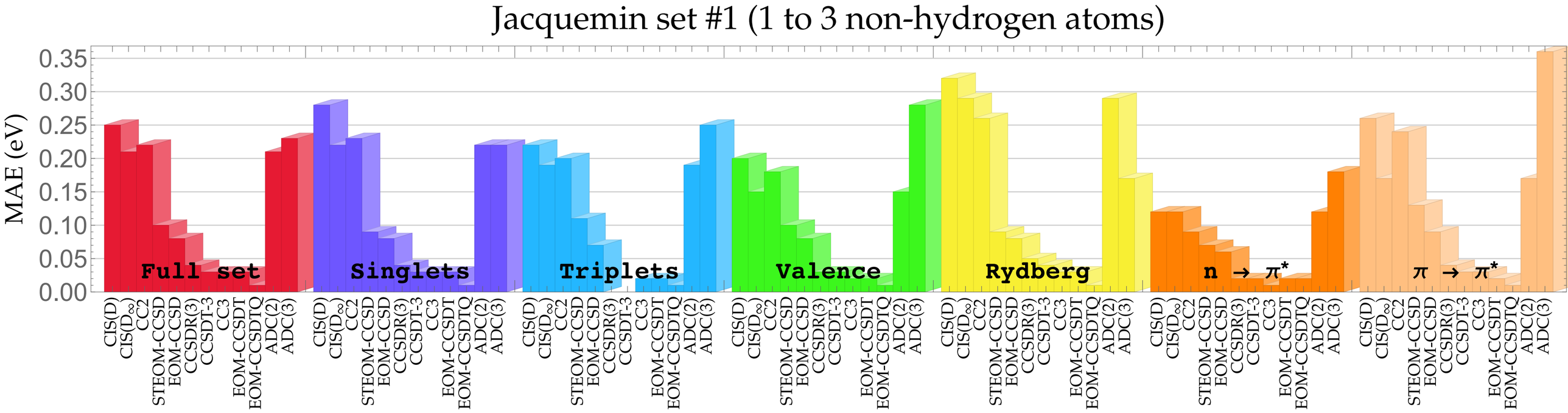
Jacquemin set #1 (1 to 3 non-hydrogen atoms)
MAE (eV)
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Full set
Singlets
Triplets
Valence
Rydberg
n → π*
π → π*
CIS(D)
CIS(D∞)
CC2
STEOM-CCSD
EOM-CCSD
CCSDR(3)
CCSDT-3
CC3
EOM-CCSDT
EOM-CCSDTQ
ADC(2)
ADC(3)