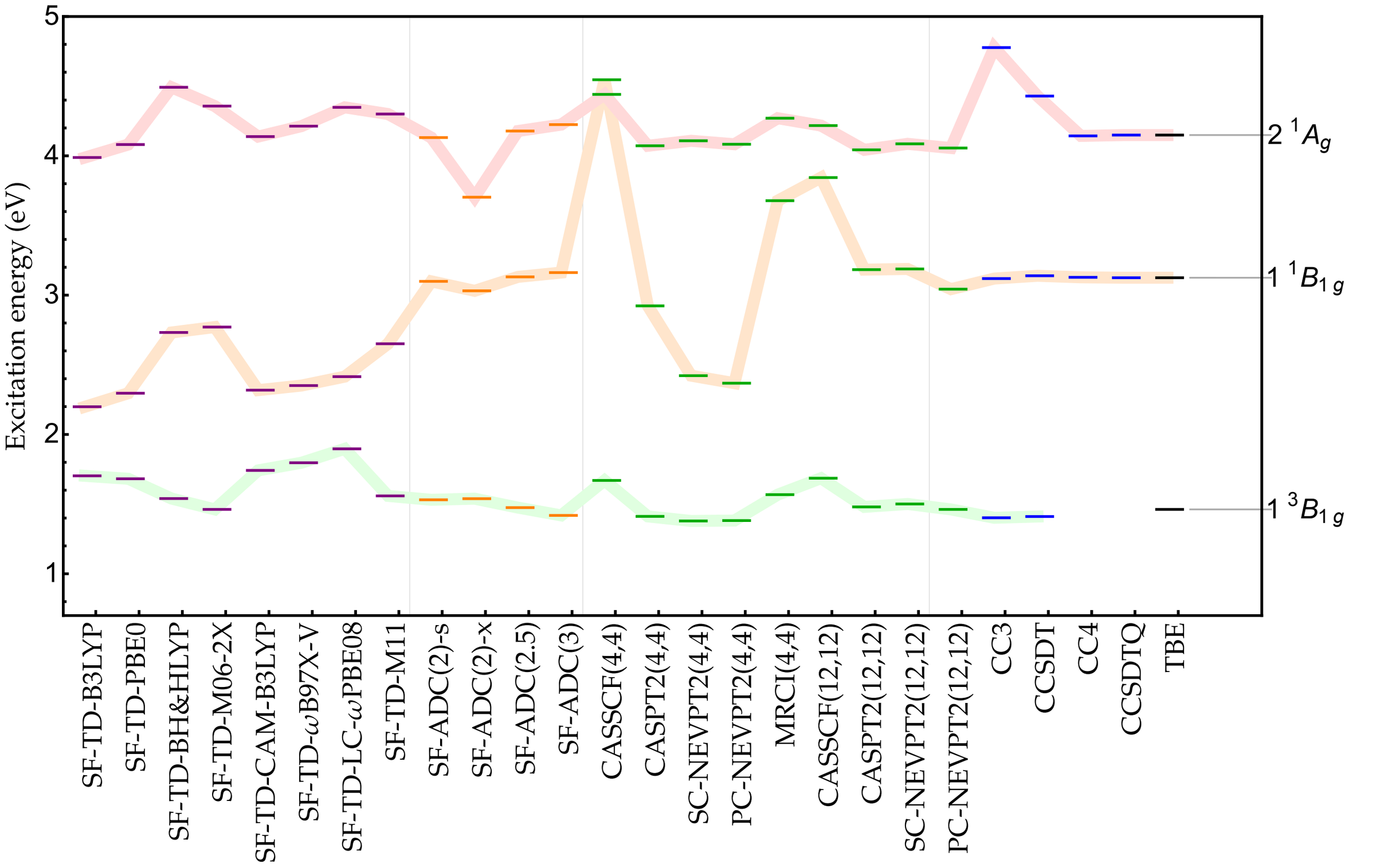
Excitation energy (eV)
5
4
3
2
1
2 ^1A_g
1 $^1B_{1g}$
1 $^3B_{1g}$
SF-TD-B3LYP
SF-TD-PBE0
SF-TD-BH&HLYP
SF-TD-M06-2X
SF-TD-CAM-B3LYP
SF-TD-ωB97X-V
SF-TD-LC-ωPBE08
SF-TD-M11
SF-ADC(2)-s
SF-ADC(2)-x
SF-ADC(2.5)
SF-ADC(3)
CASSCF(4,4)
CASPT2(4,4)
SC-NEVPT2(4,4)
PC-NEVPT2(4,4)
MRCI(4,4)
CASSCF(12,12)
CASPT2(12,12)
SC-NEVPT2(12,12)
PC-NEVPT2(12,12)
CC3
CCSDT
CC4
CCSDTQ
TBE