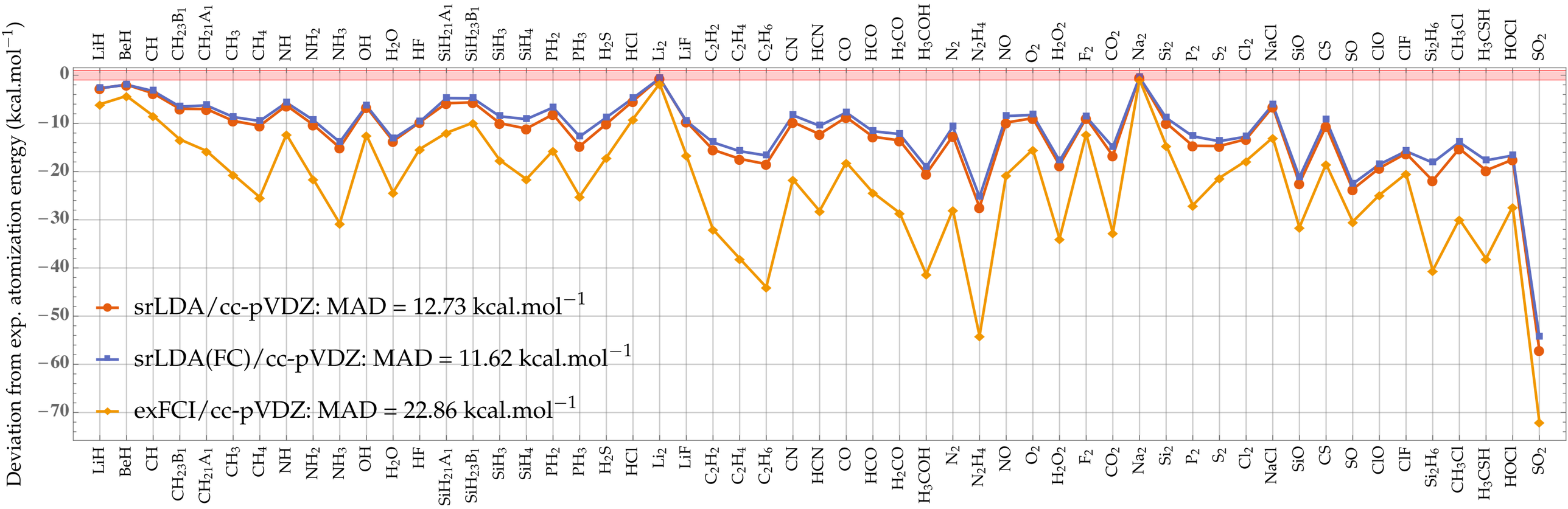
Deviation from exp. atomization energy (kcal.mol^{-1})
0
−10
−20
−30
−40
−50
−60
−70
srLDA/cc-pVDZ: MAD = 12.73 kcal.mol^{-1}
srLDA(FC)/cc-pVDZ: MAD = 11.62 kcal.mol^{-1}
exFCI/cc-pVDZ: MAD = 22.86 kcal.mol^{-1}
LiH
BeH
CH
$CH_2{}^3B_1$
$CH_2{}^1A_1$
CH_3
CH_4
NH
NH_2
NH_3
OH
H_2O
HF
$SiH_2{}^1A_1$
$SiH_2{}^3B_1$
SiH_3
SiH_4
PH_2
PH_3
H_2S
HCl
Li_2
LiF
C_2H_2
C_2H_4
C_2H_6
CN
HCN
CO
HCO
H_2CO
H_3COH
N_2
N_2H_4
NO
O_2
H_2O_2
F_2
CO_2
Na_2
Si_2
P_2
S_2
Cl_2
NaCl
SiO
CS
SO
ClO
ClF
Si_2H_6
CH_3Cl
H_3CSH
HOCl
SO_2