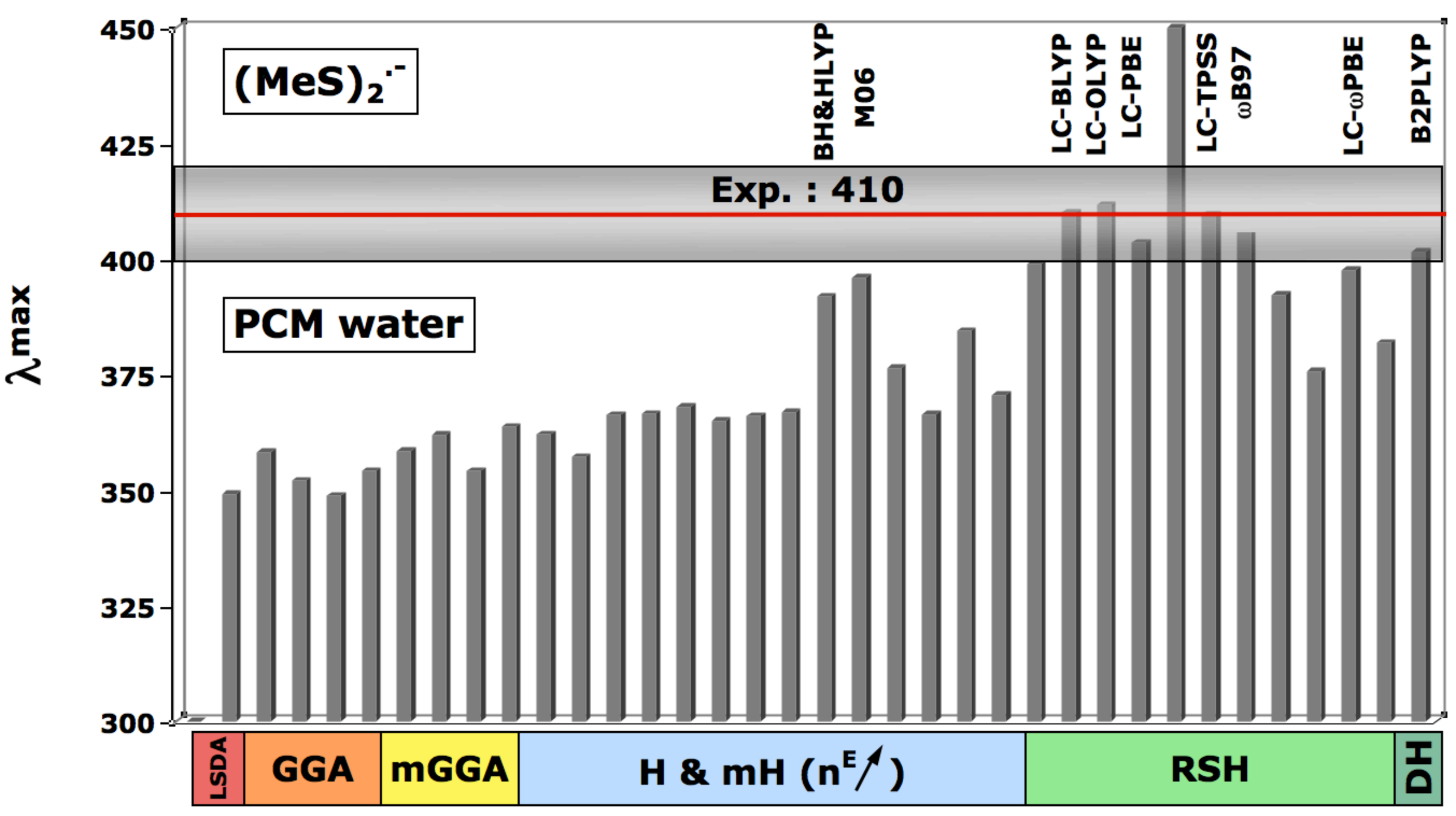
(MeS)2·-
PCM water
Exp. : 410
λmax
450
425
400
375
350
325
300
BH&HLYP
M06
LC-BLYP
LC-OLYP
LC-PBE
LC-TPSS
ωB97
LC-ωPBE
B2PLYP
LSDA
GGA
mGGA
H & mH (nE↗)
RSH
DH