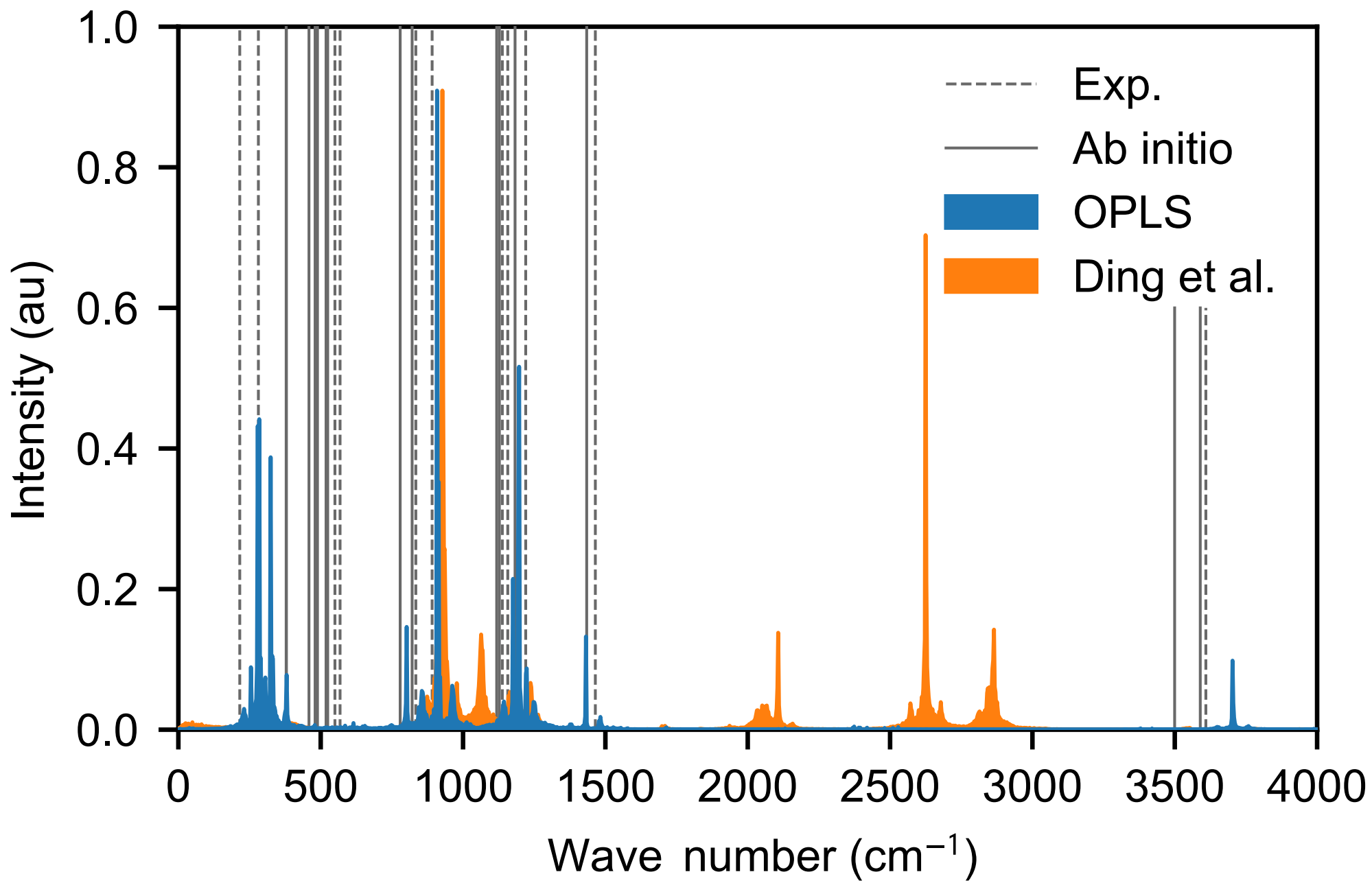
Exp.
Ab initio
OPLS
Ding et al.
Intensity (au)
Wave number (cm^{-1})
0.0
0.2
0.4
0.6
0.8
1.0
0
500
1000
1500
2000
2500
3000
3500
4000