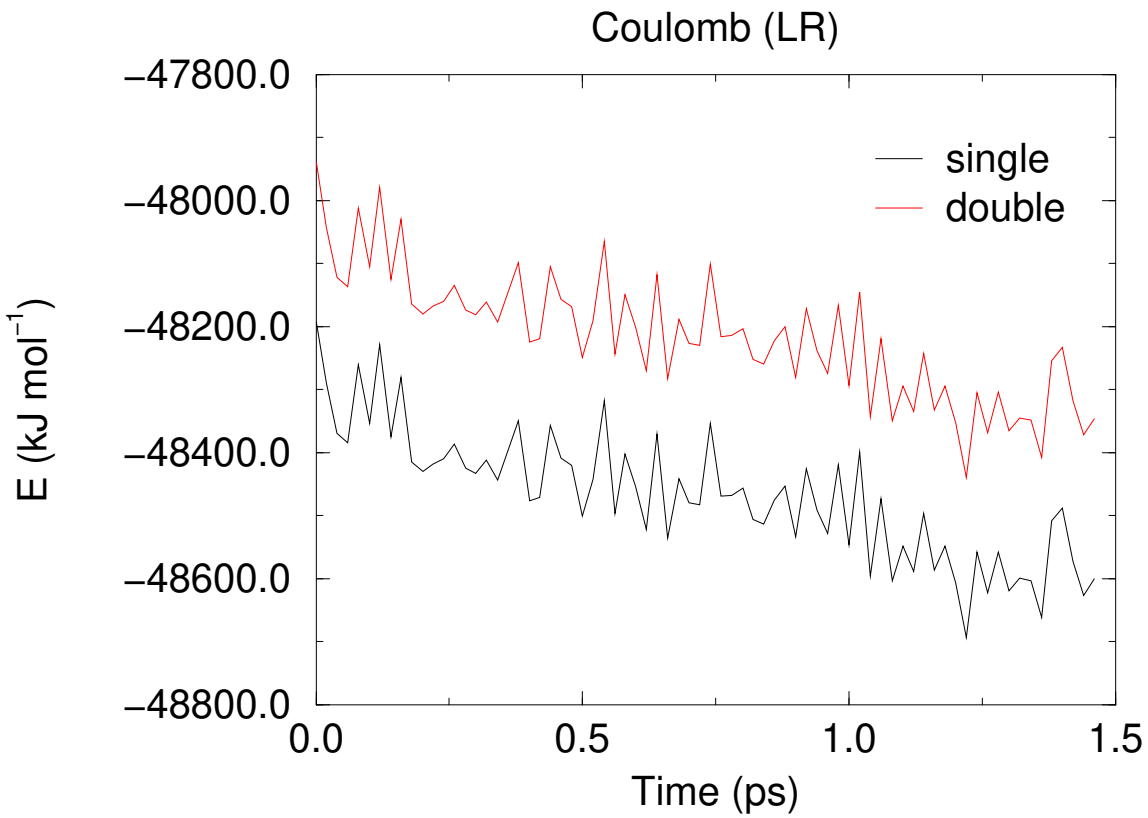
Coulomb (LR)
−47800.0
−48000.0
−48200.0
−48400.0
−48600.0
−48800.0
E (kJ mol^{-1})
0.0
0.5
1.0
1.5
Time (ps)
single
double