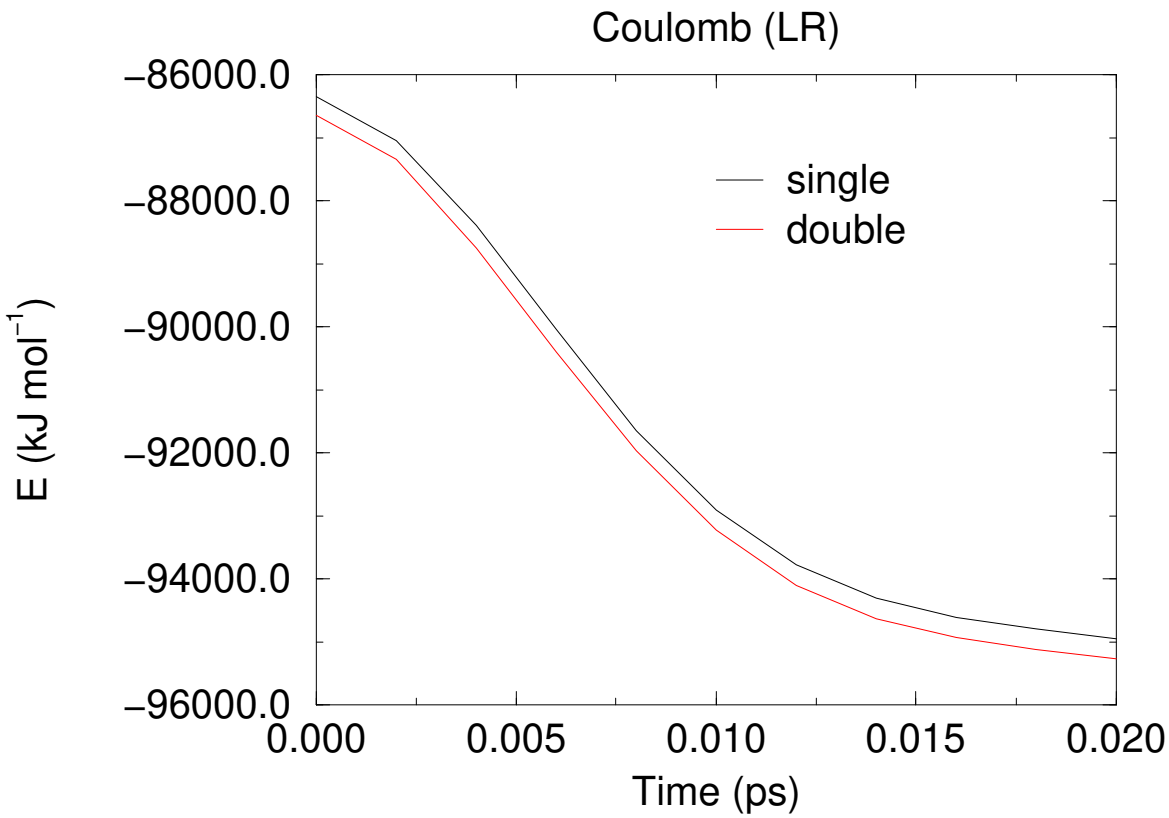
Coulomb (LR)
−86000.0
−88000.0
−90000.0
−92000.0
−94000.0
−96000.0
E (kJ mol^{-1})
0.000
0.005
0.010
0.015
0.020
Time (ps)
single
double