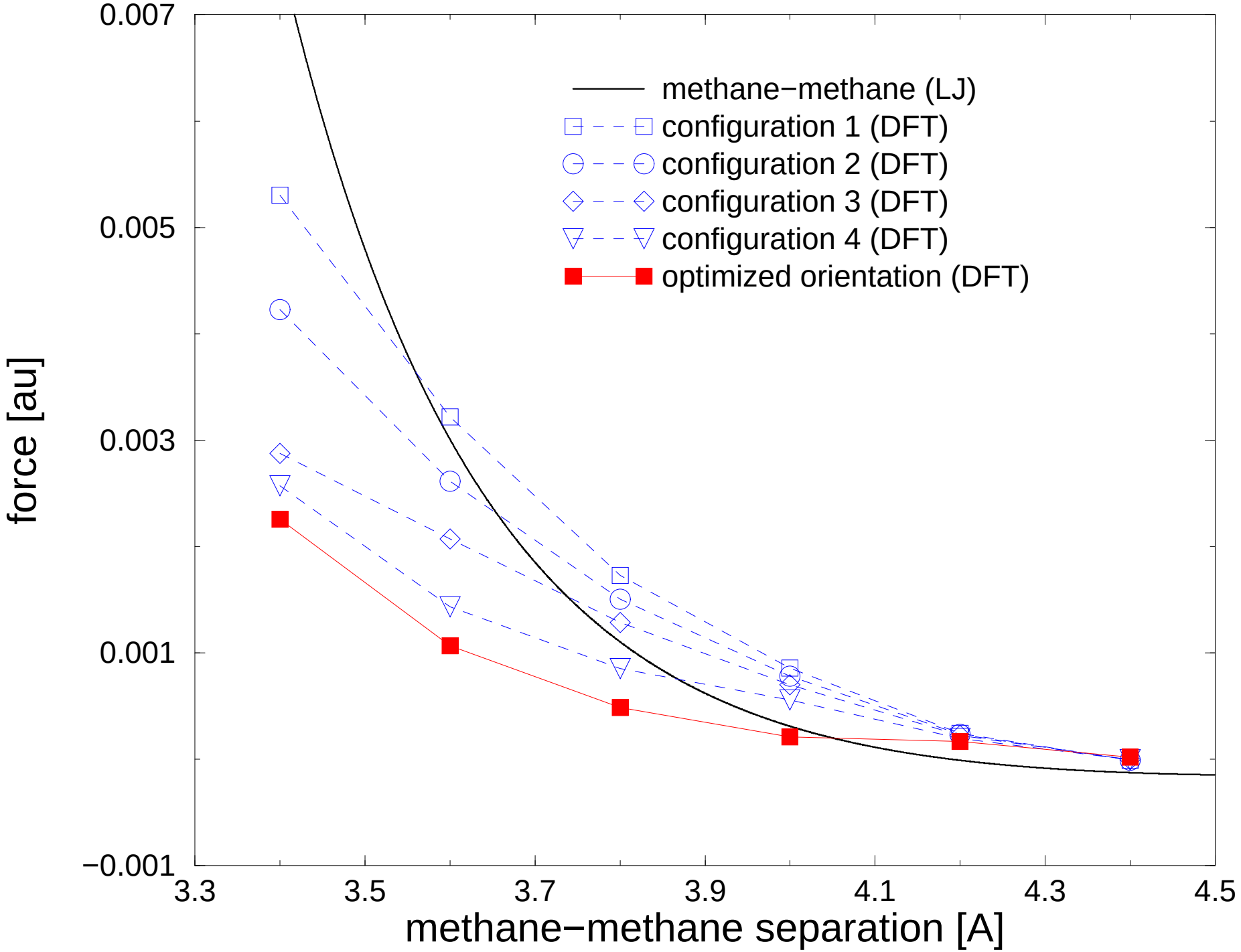
methane−methane (LJ)
configuration 1 (DFT)
configuration 2 (DFT)
configuration 3 (DFT)
configuration 4 (DFT)
optimized orientation (DFT)
force [au]
methane−methane separation [A]
0.007
0.005
0.003
0.001
−0.001
3.3
3.5
3.7
3.9
4.1
4.3
4.5