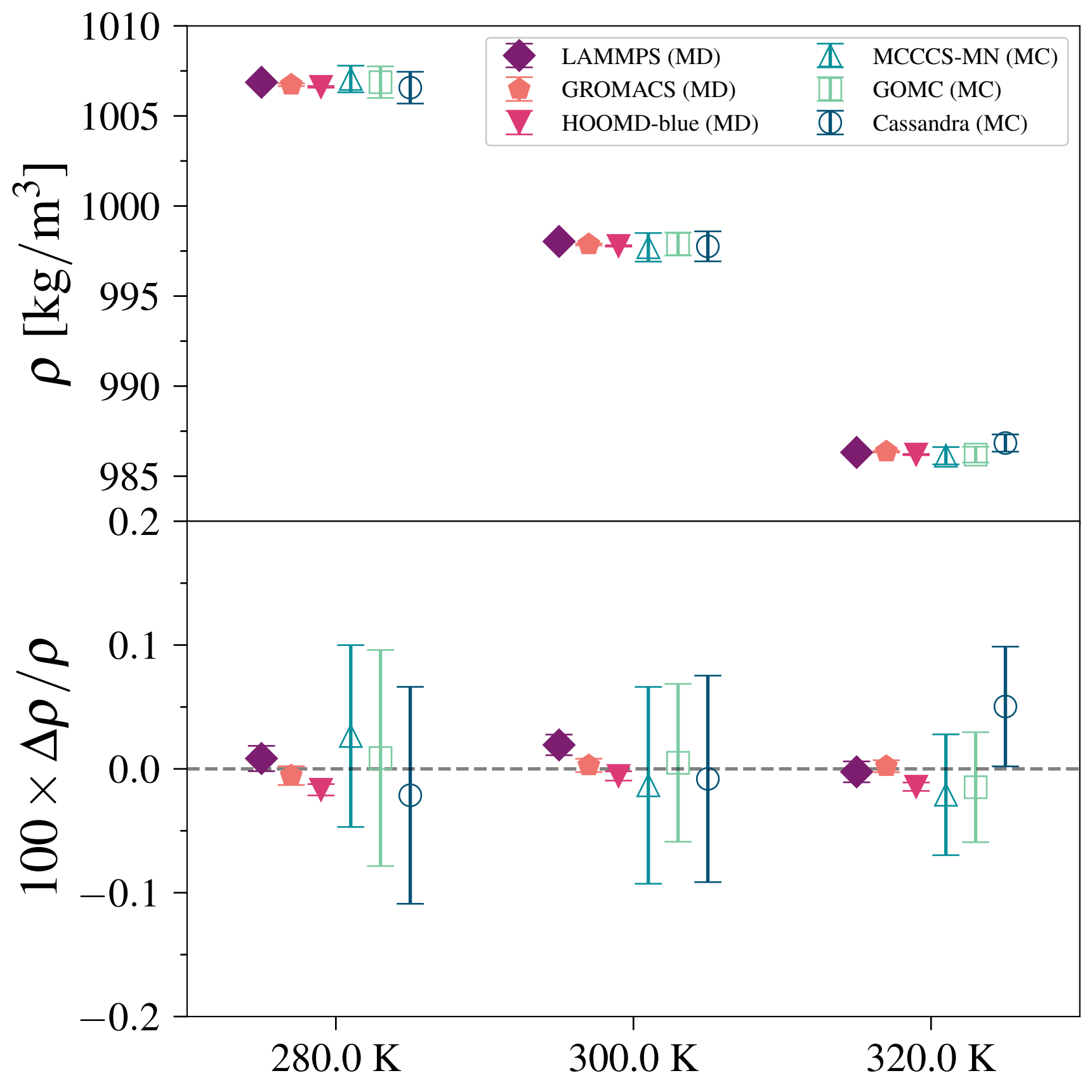
LAMMPS (MD)
GROMACS (MD)
HOOMD-blue (MD)
MCCCS-MN (MC)
GOMC (MC)
Cassandra (MC)
ρ [kg/m³]
1010
1005
1000
995
990
985
100 × Δρ/ρ
0.2
0.1
0.0
−0.1
−0.2
280.0 K
300.0 K
320.0 K