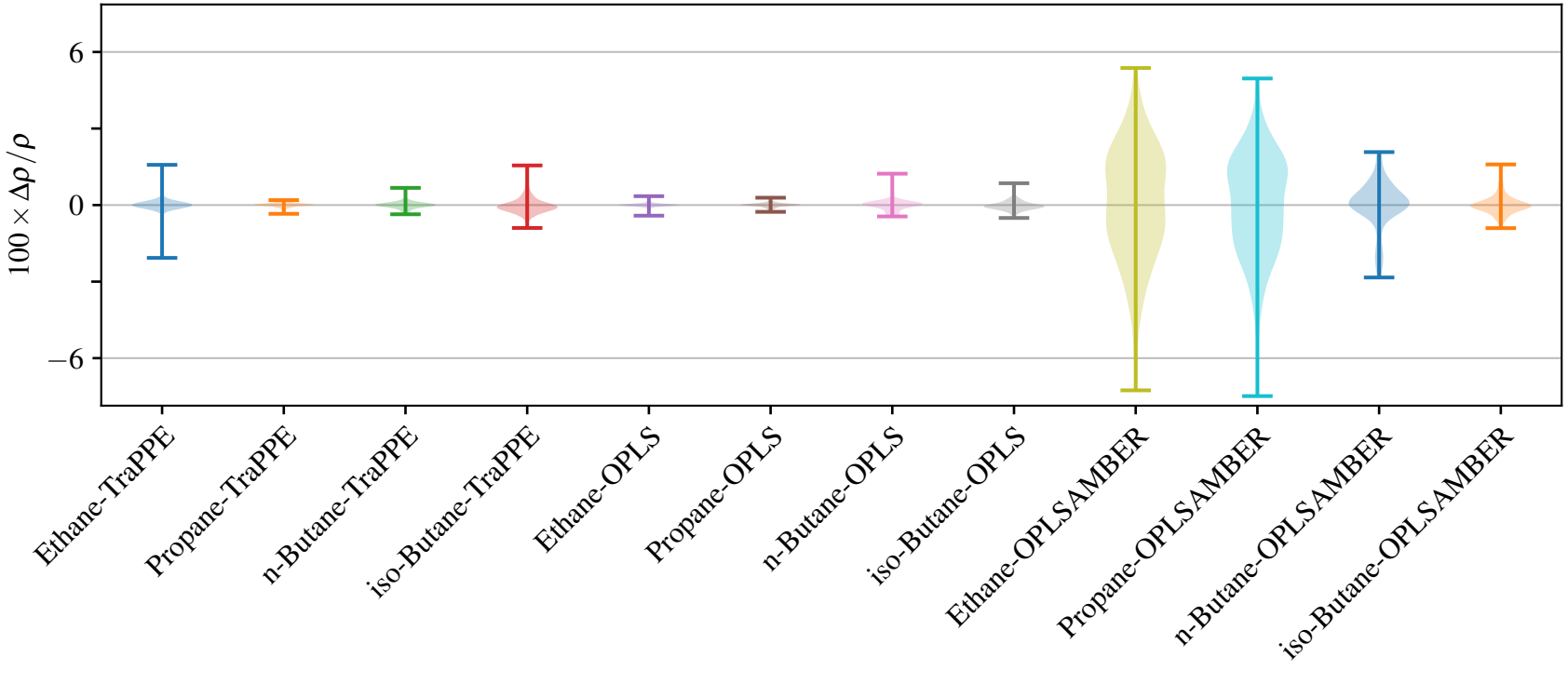
6
0
−6
$100 \times \Delta\rho/\rho$
Ethane-TraPPE
Propane-TraPPE
n-Butane-TraPPE
iso-Butane-TraPPE
Ethane-OPLS
Propane-OPLS
n-Butane-OPLS
iso-Butane-OPLS
Ethane-OPLSAMBER
Propane-OPLSAMBER
n-Butane-OPLSAMBER
iso-Butane-OPLSAMBER