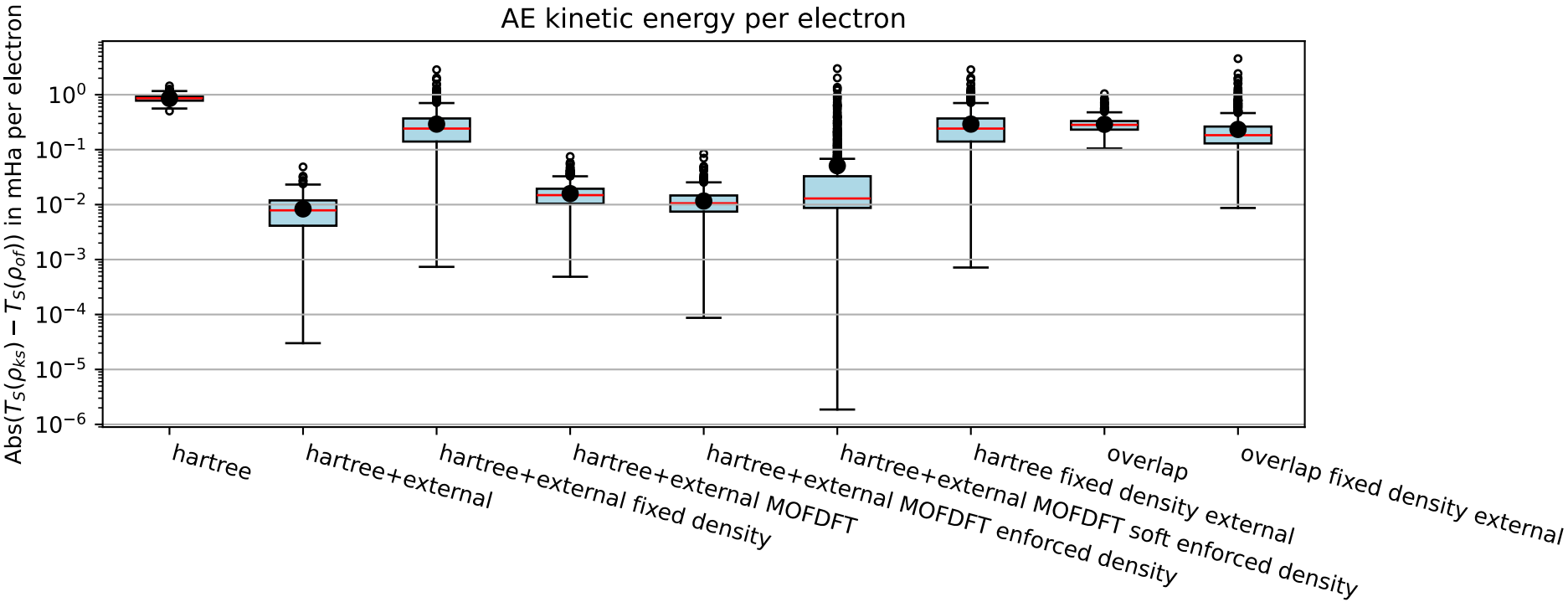
AE kinetic energy per electron
Abs($T_S(\rho_{ks}) - T_S(\rho_{of})$) in mHa per electron
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
hartree
hartree+external
hartree+external fixed density
hartree+external MOFDFT
hartree+external MOFDFT enforced density
hartree+external MOFDFT soft enforced density
hartree fixed density external
overlap
overlap fixed density external