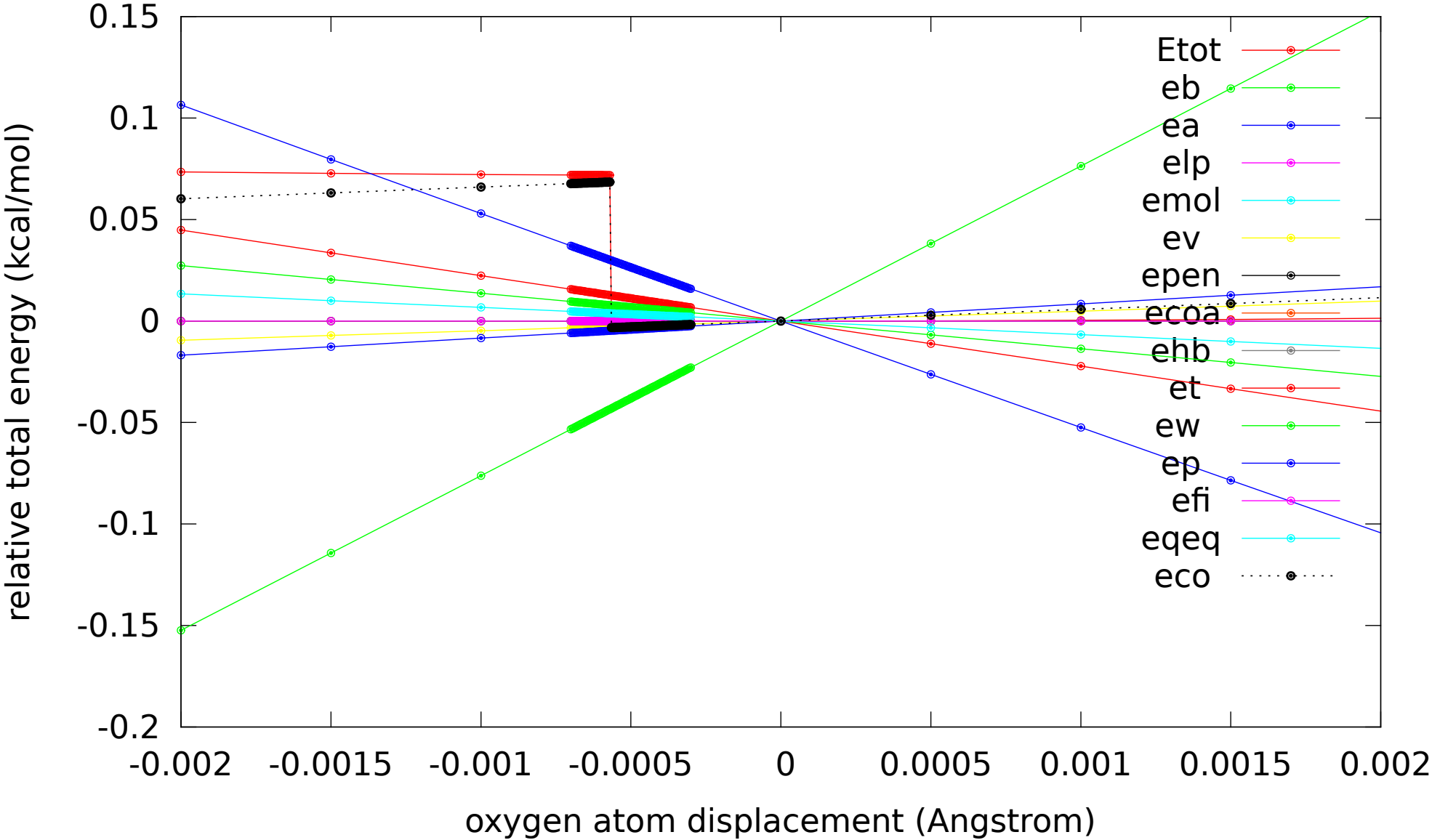
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
relative total energy (kcal/mol)
-0.002
-0.0015
-0.001
-0.0005
0
0.0005
0.001
0.0015
0.002
oxygen atom displacement (Angstrom)
Etot
eb
ea
elp
emol
ev
epen
ecoa
ehb
et
ew
ep
efi
eqeq
eco