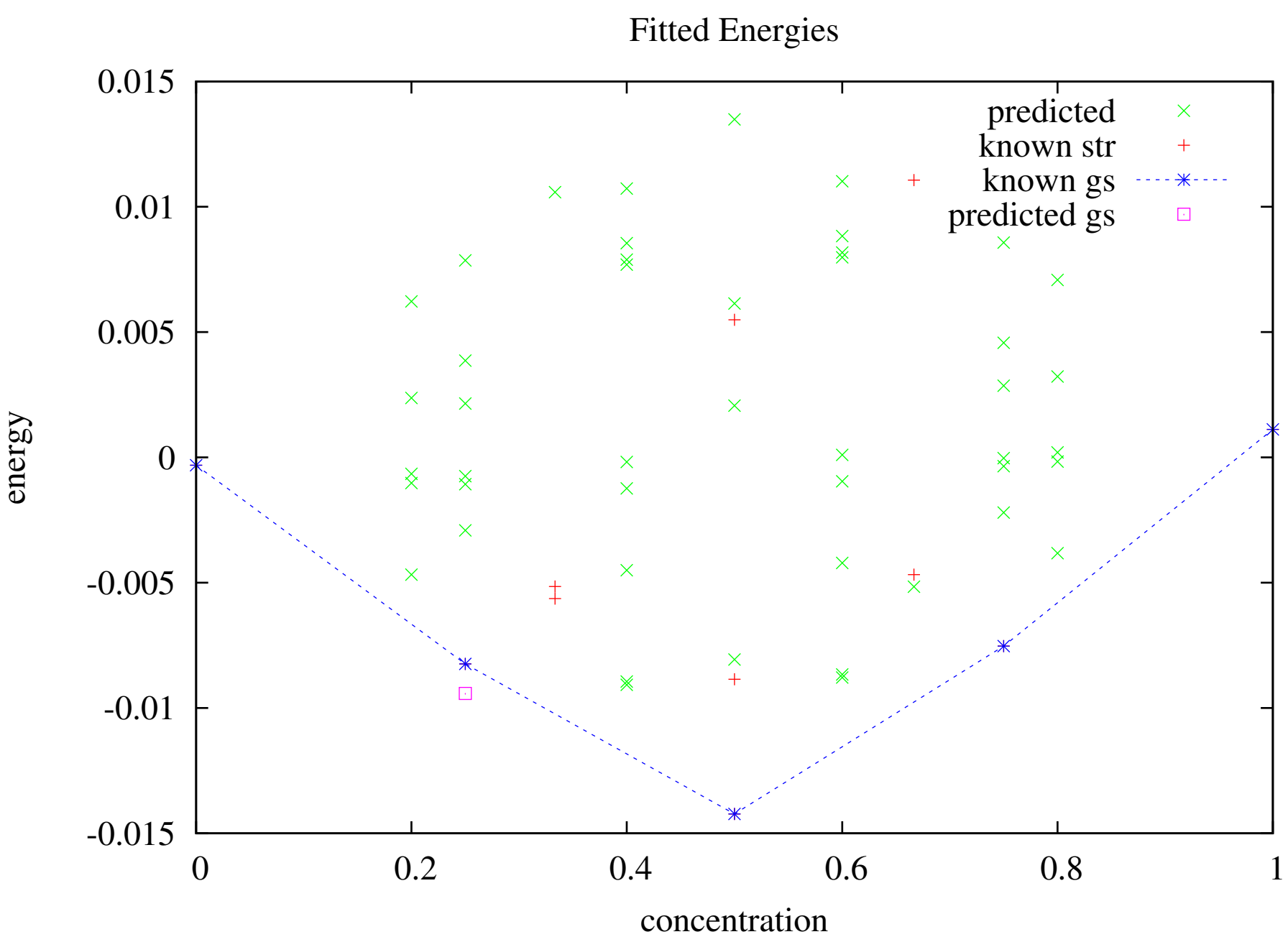
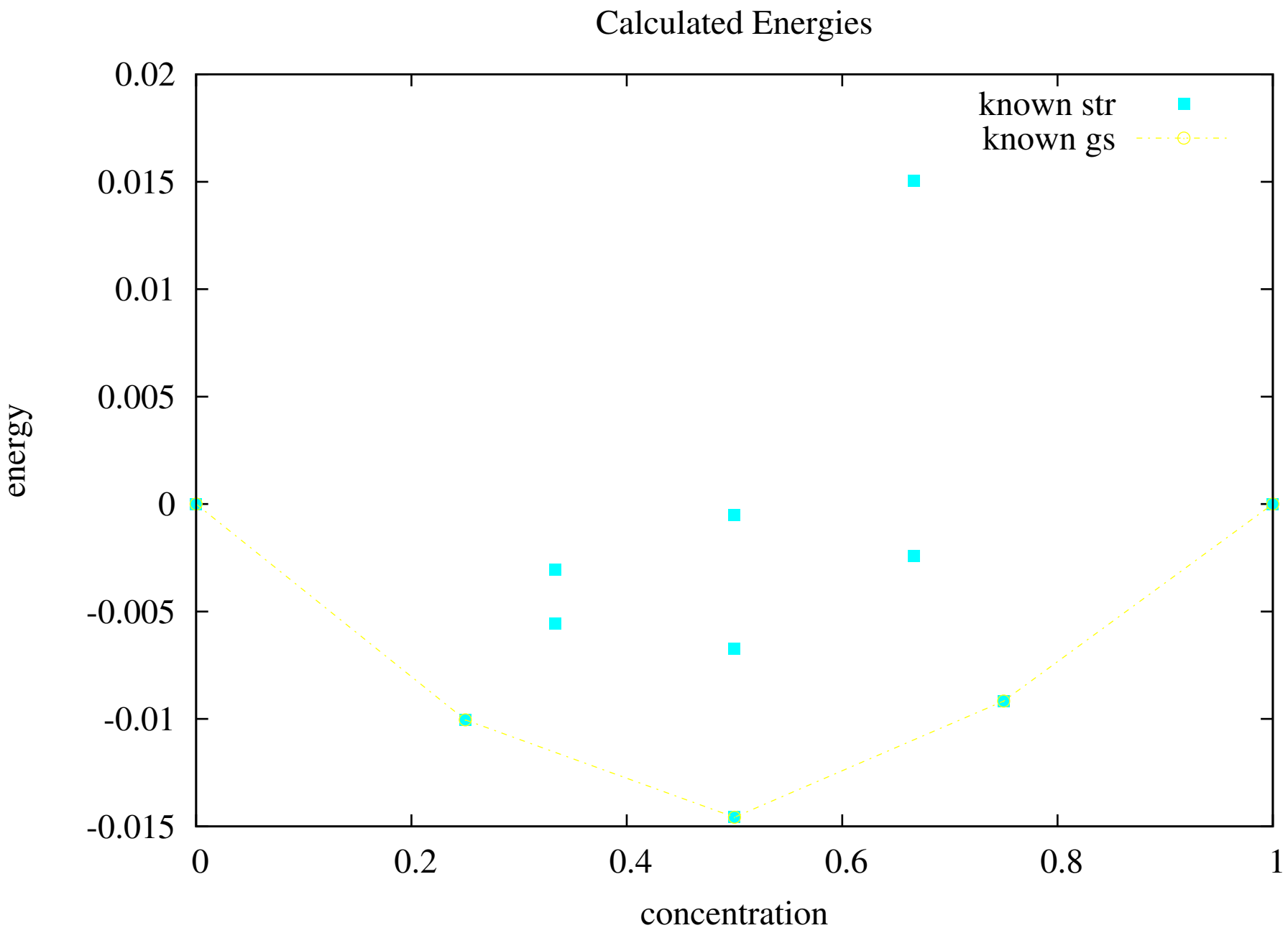
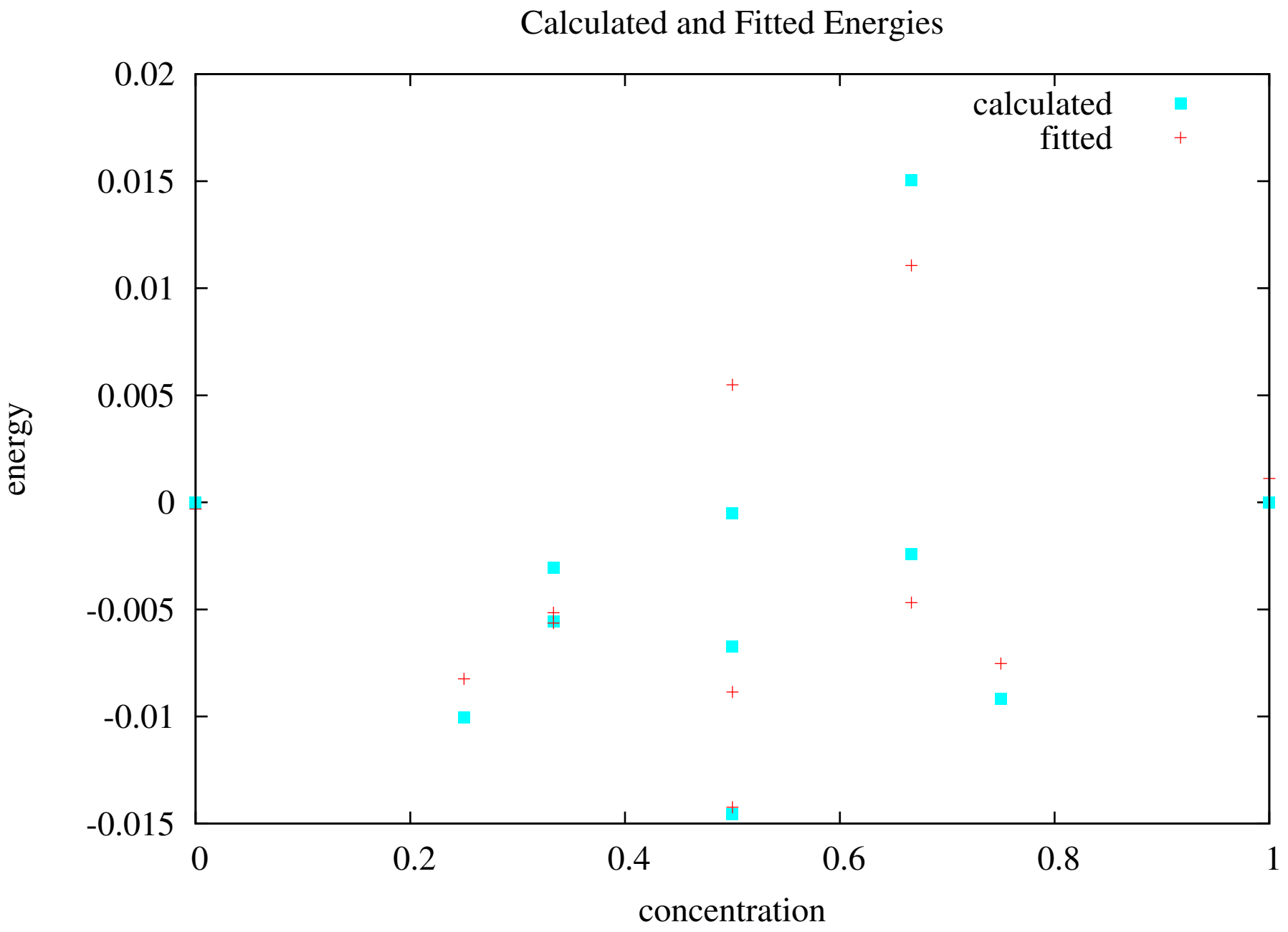
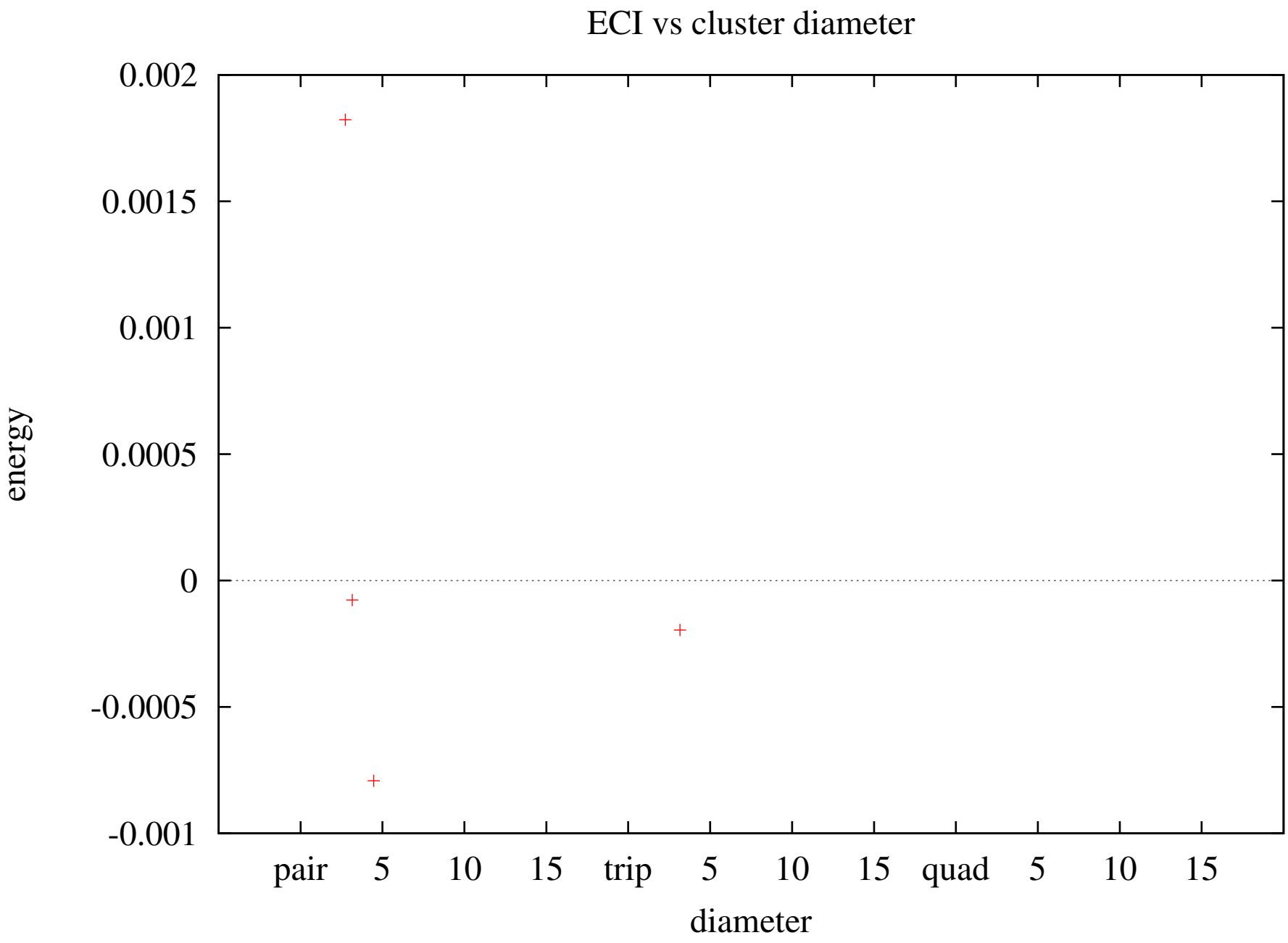
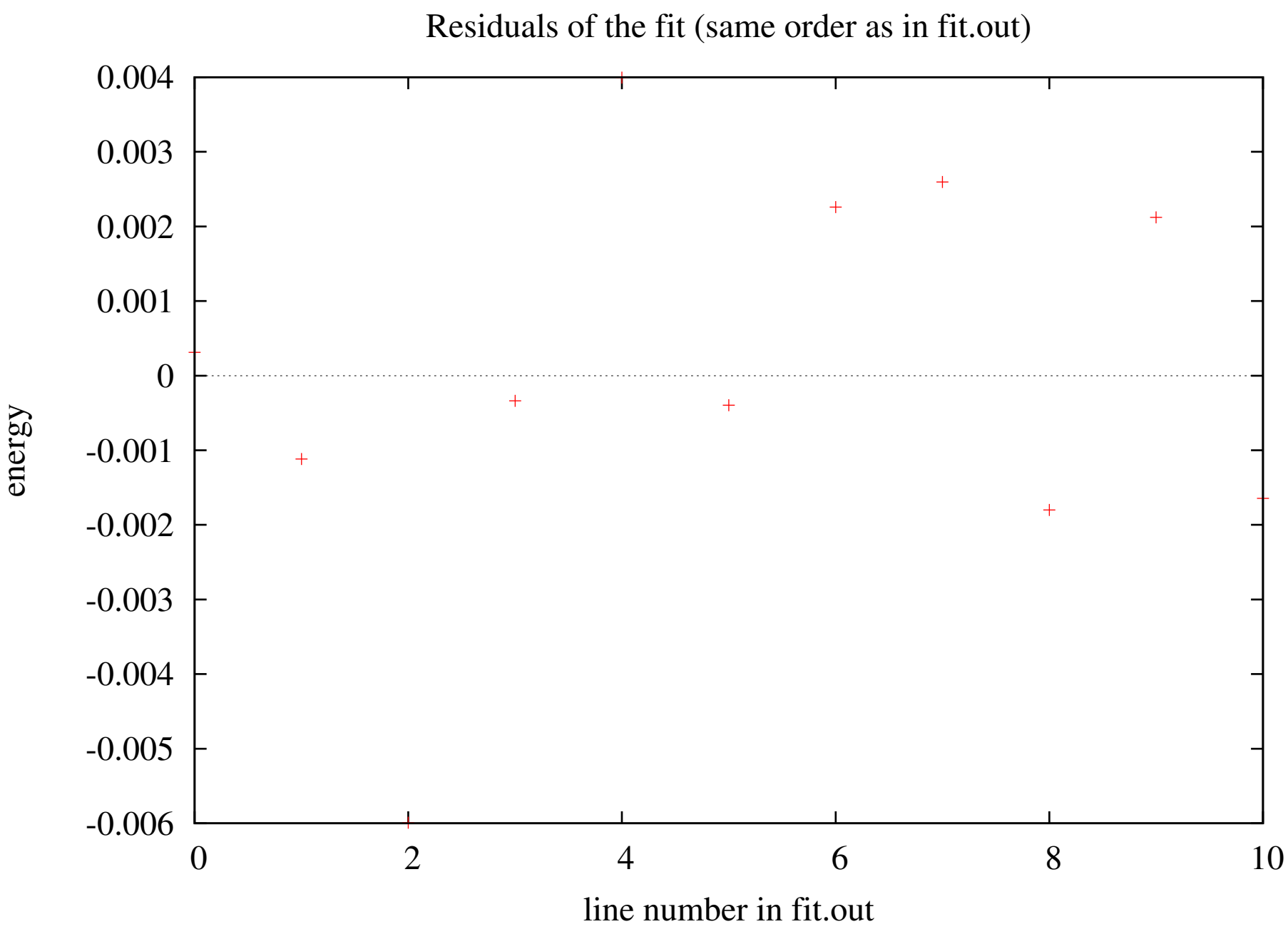
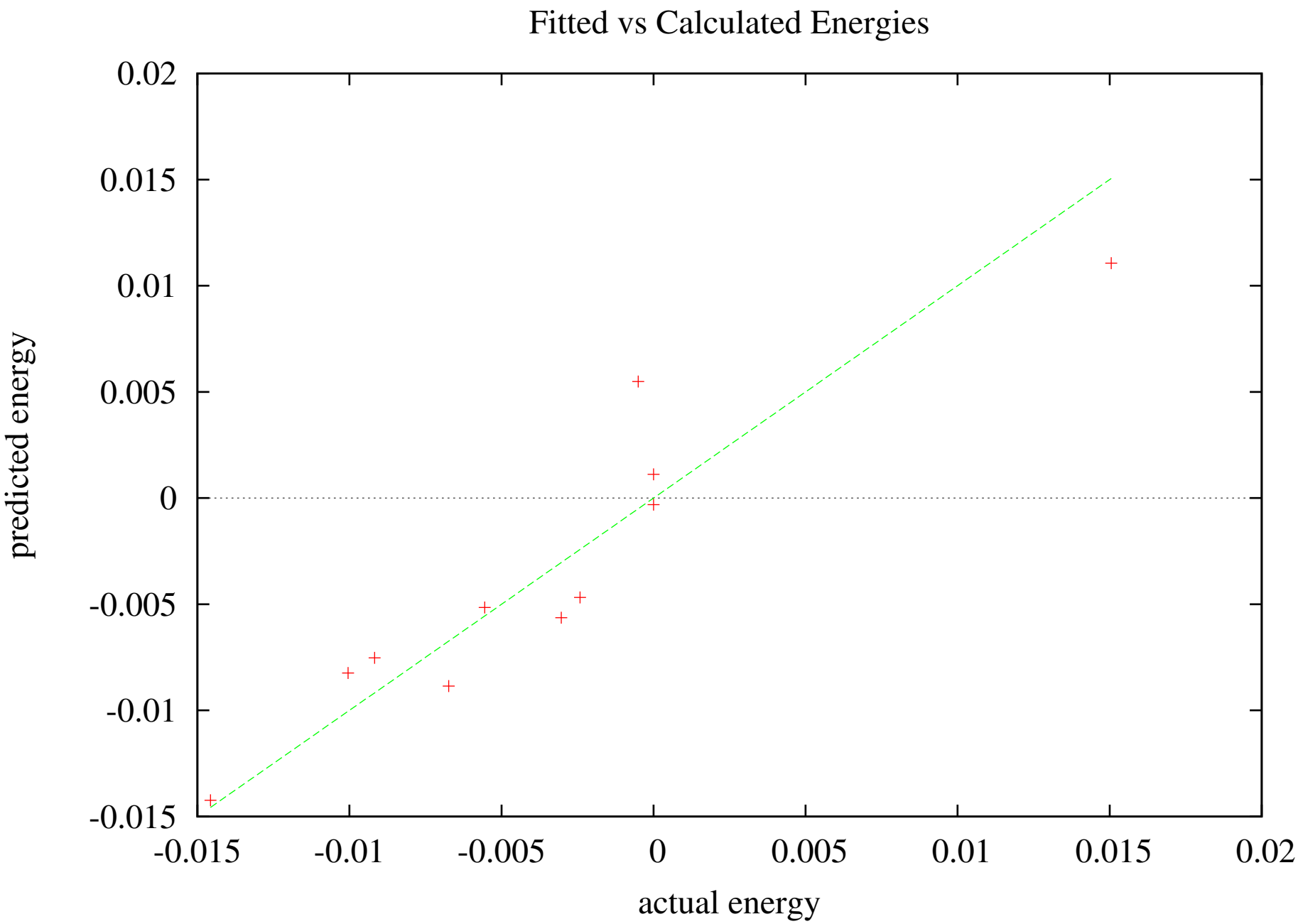

Fitted Energies
predicted
known str
known gs
predicted gs
energy
concentration
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
0
0.2
0.4
0.6
0.8
1


Calculated Energies
known str
known gs
energy
concentration
0.02
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
0
0.2
0.4
0.6
0.8
1


Calculated and Fitted Energies
calculated
fitted
energy
concentration
0.02
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
0
0.2
0.4
0.6
0.8
1


ECI vs cluster diameter
0.002
0.0015
0.001
0.0005
0
-0.0005
-0.001
energy
pair
5
10
15
trip
5
10
15
quad
5
10
15
diameter


Residuals of the fit (same order as in fit.out)
0.004
0.003
0.002
0.001
0
-0.001
-0.002
-0.003
-0.004
-0.005
-0.006
energy
0
2
4
6
8
10
line number in fit.out


Fitted vs Calculated Energies
predicted energy
actual energy
0.02
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
-0.015
-0.01
-0.005
0
0.005
0.01
0.015
0.02