

Result

Task started: 20:10 02-07-2017
Task ended: 20:10 02-07-2017
Total time consumed: 0 min on 64 tasks

Control

XC	pbe
Relativistic	atomic_zora
Charge	1
Max. number of iterations is	1000
Relaxation was performed	

Other settings:

vdw_correction_hirshfeld
sc_accuracy_rho 1E-3
sc_accuracy_eev 1E-2
sc_accuracy_etot 1E-5
sc_accuracy_forces 5E-3

Figure 1: Atoms: H, O, C, N, Na, Ca

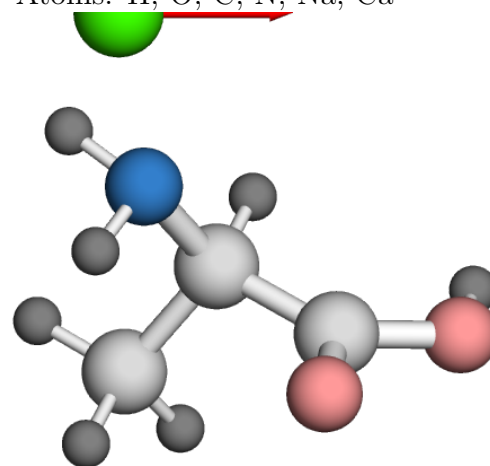


Figure 2: Energy convergence during geometry relaxation process.

