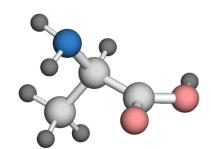
Result

Task started: 20:29 02-07-2017
Task ended: 20:30 02-07-2017
Total time consumed: 1 min on 64 tasks

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



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 check_cpu_consistency .false. cpu_consistency_threshold 5E-3

Figure 2: Energy convergence during geometry relaxation process.

