



Solutions

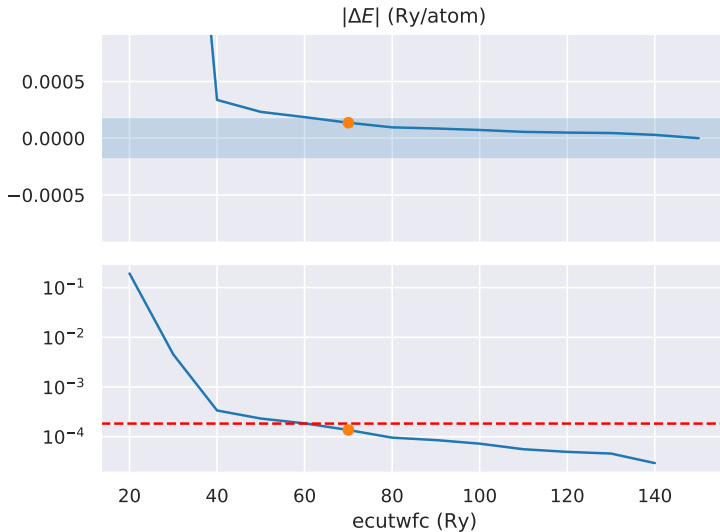
Convergence of energy and forces, calculating bulk modulus, and elastic constants of NaCl

Edward Linscott

Quantum Espresso Workshop, Virtual Winterschool in Chemistry, 19 Feb 2021

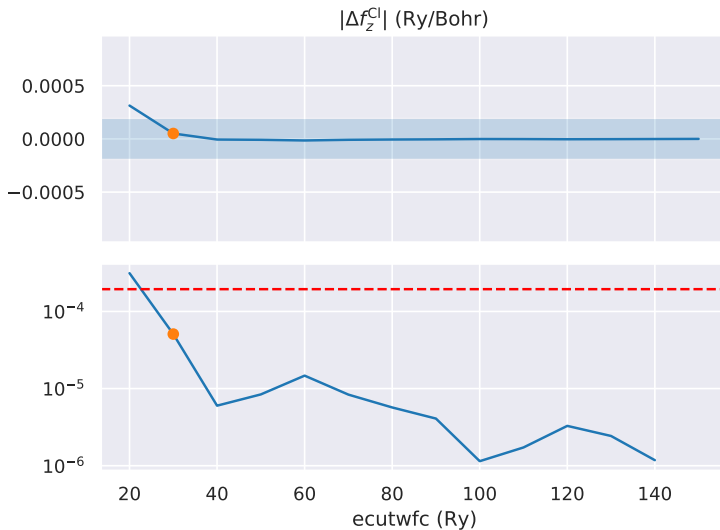
Exercise 1: convergence

Total energy with respect to energy cutoff



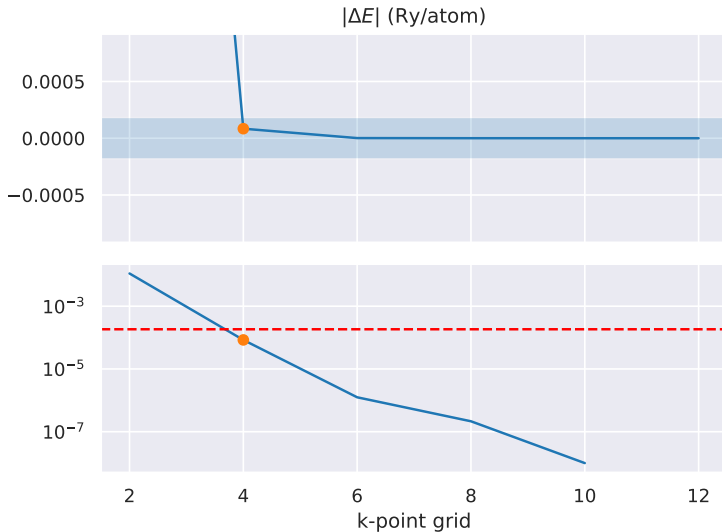
Exercise 1: convergence

Forces with respect to energy cutoff



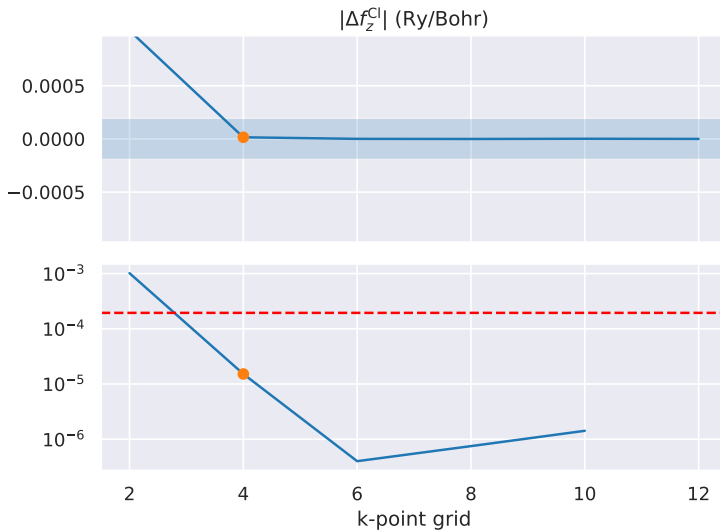
Exercise 1: convergence

Energy with respect to k-point grid



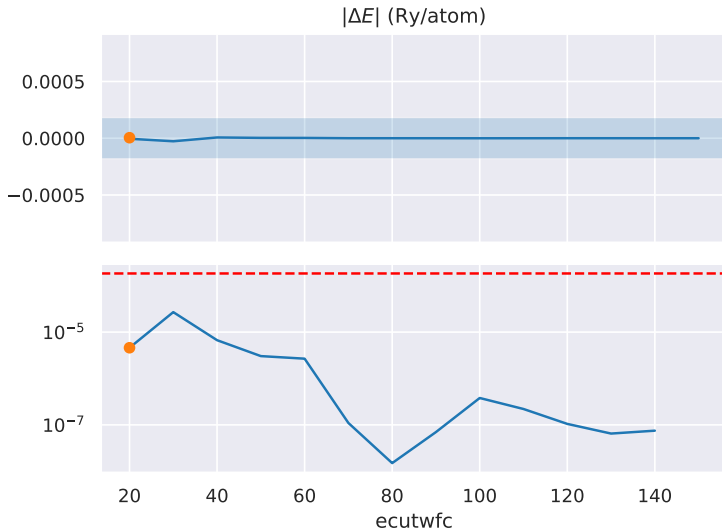
Exercise 1: convergence

Forces with respect to k-point grid



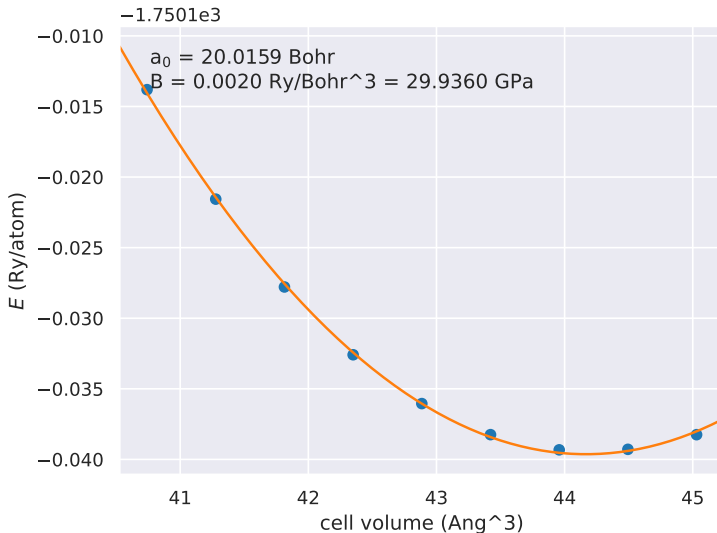
Exercise 1: convergence

Energy differences with respect to energy cutoff



Exercise 2: calculating the bulk modulus

Parabolic fit



Exercise 2: calculating the bulk modulus

Birch Murnaghan fit

