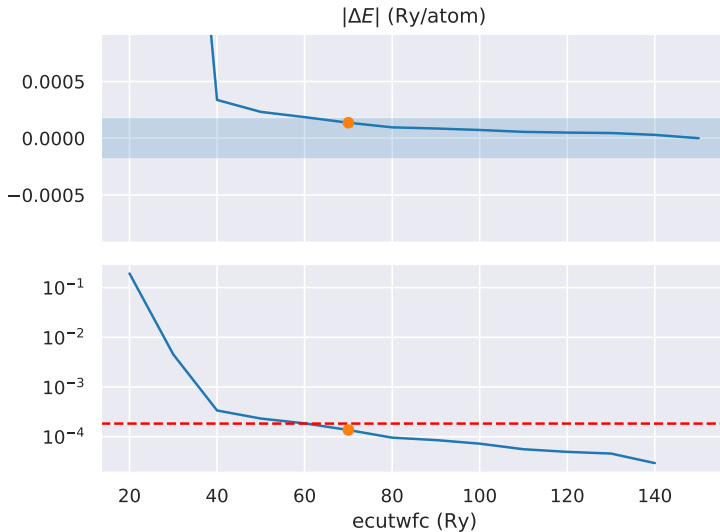# Solutions
**Convergence of energy and forces, calculating bulk modulus, and elastic constants of NaCl**

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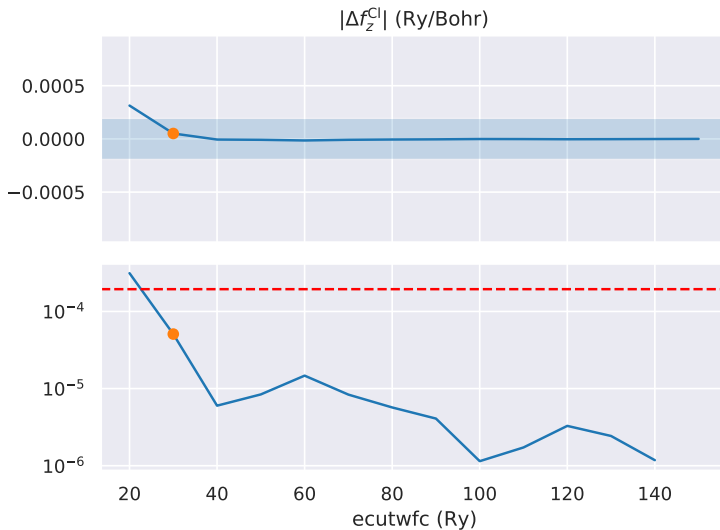Quantum Espresso Workshop, Virtual Winterschool in Chemistry, 19 Feb 2021

# Exercise 1: convergence
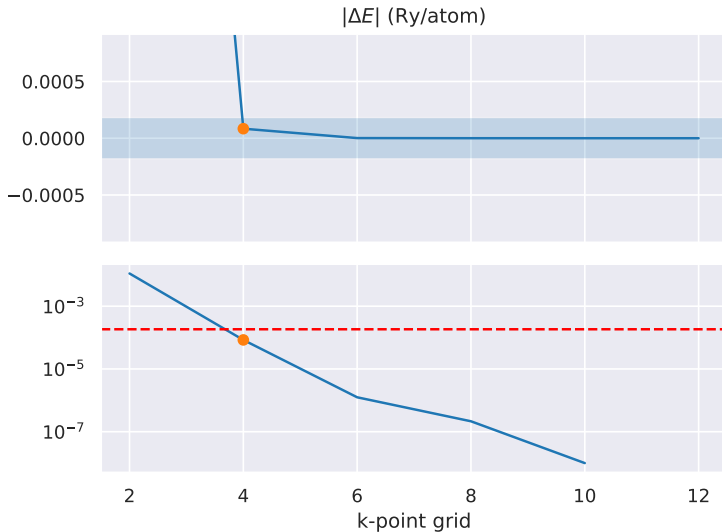
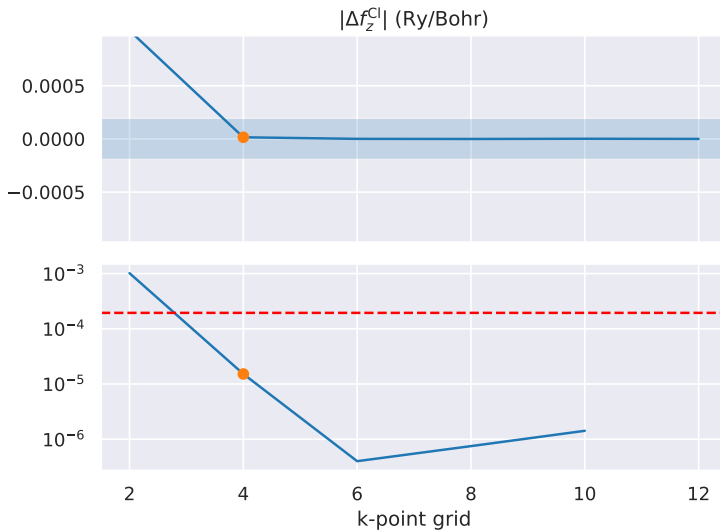Total energy with respect to energy cutoff

Forces with respect to energy cutoff



$|\Delta f_z^{Cl}|$ (Ry/Bohr)

# Exercise 1: convergence

Energy with respect to k-point grid

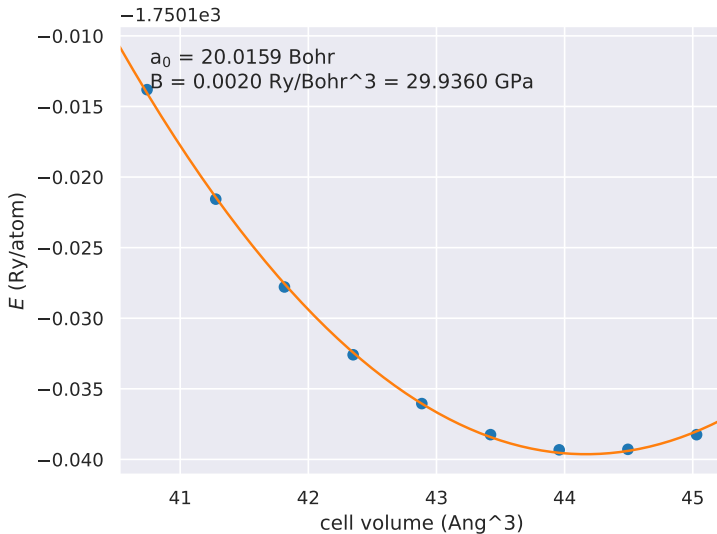# Exercise 1: convergence

Forces with respect to k-point grid



$|\Delta f_z^{Cl}|$ (Ry/Bohr)

# Exercise 1: convergence
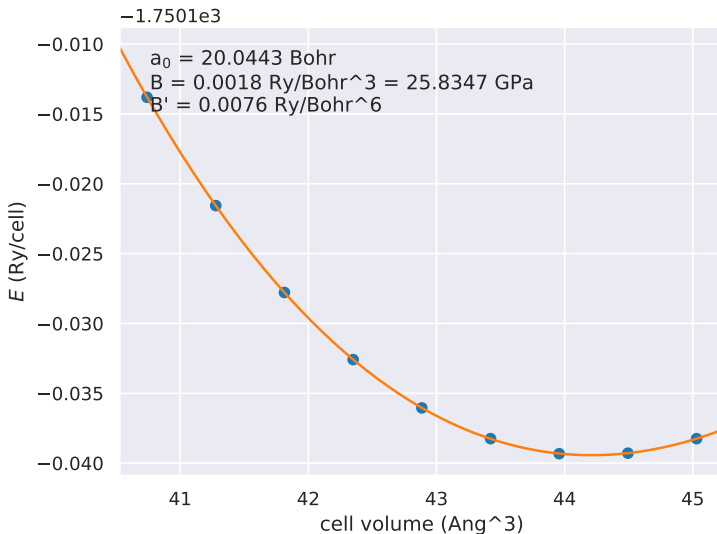
Energy differences with respect to energy cutoff



$|\Delta E|$ (Ry/atom)
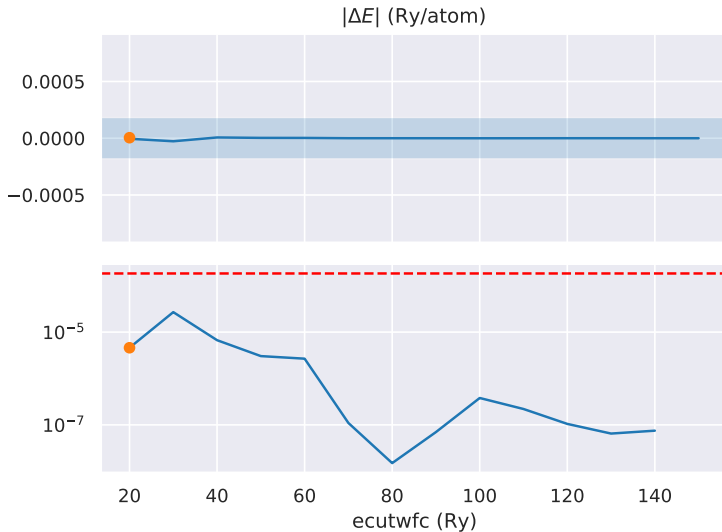
# Exercise 2: calculating the bulk modulus

Parabolic fit

# Exercise 2: calculating the bulk modulus

Birch Murnaghan fit



$a_0$ = 20.0443 Bohr
B = 0.0018 Ry/Bohr^3 = 25.8347 GPa
B' = 0.0076 Ry/Bohr^6

# Exercise 3: elastic constants

## Orthorhombic distortion



$C_{11} = 0.0037$ Ry/Bohr^3 = 54.7821 GPa
$C_{12} = 0.0008$ Ry/Bohr^3 = 11.3611 GPa
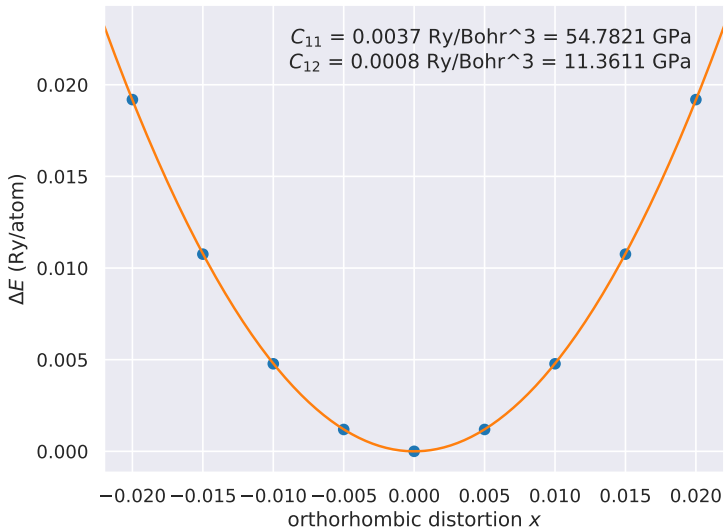
# Exercise 3: elastic constants

## Monoclinic distortion