Supporting Information for:

Optimizing a parametrized Thomas-Fermi-Dirac-Weizsäcker functional for atoms

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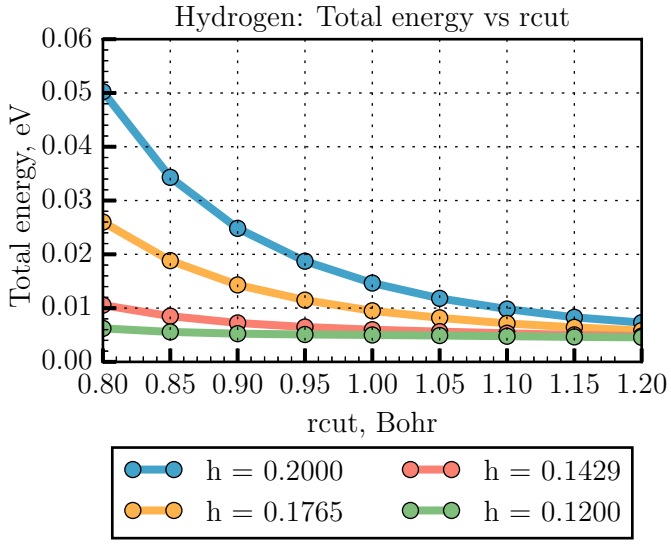
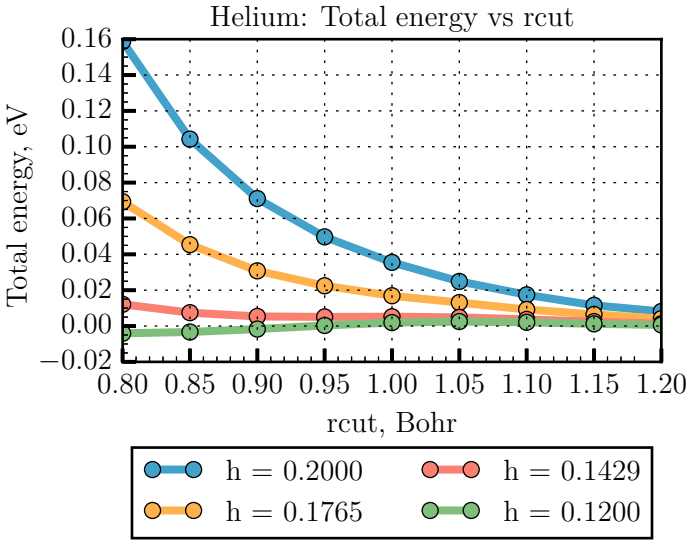
This supporting information was prepared on Feb. 27, 2015 and consists of a total of 4 pages. Prepared for PCCP. Convergency benchmark for the first and second row elements of the periodic table.

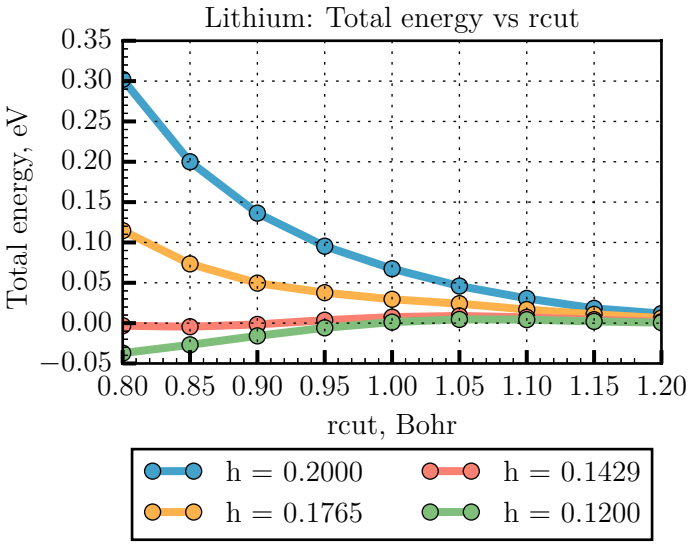
Contents:

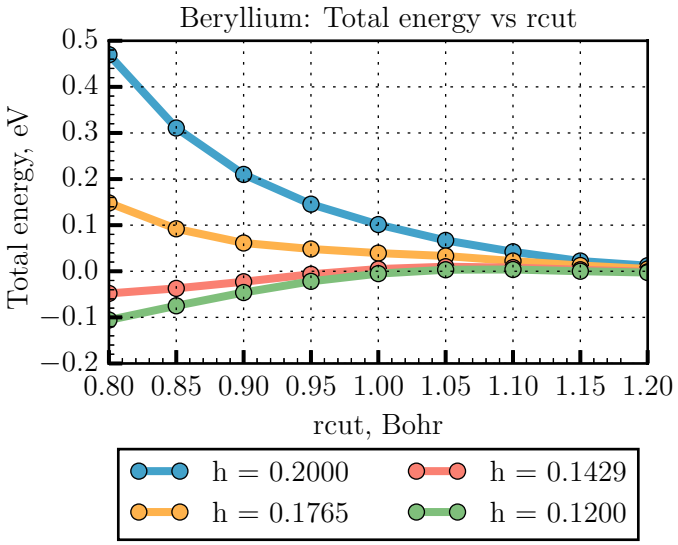
1. Variation of rcut values for the atoms.

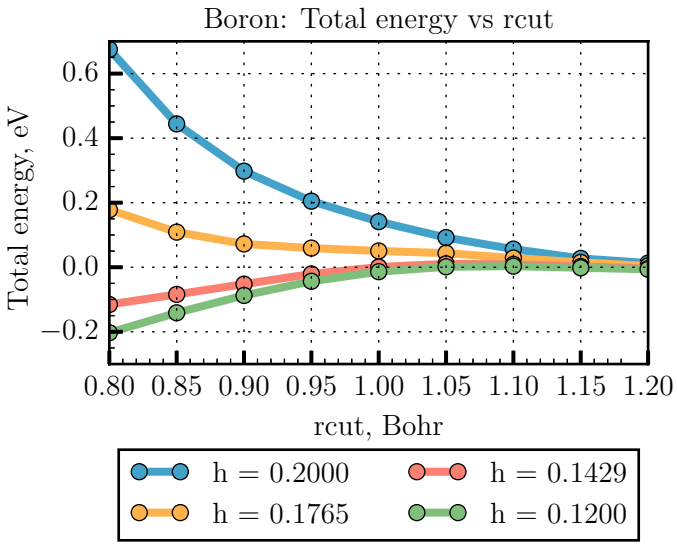
The input parameters to be used: lambda = 1.0, gamma = 1.0, mix = 0.01, gpernode = 800.

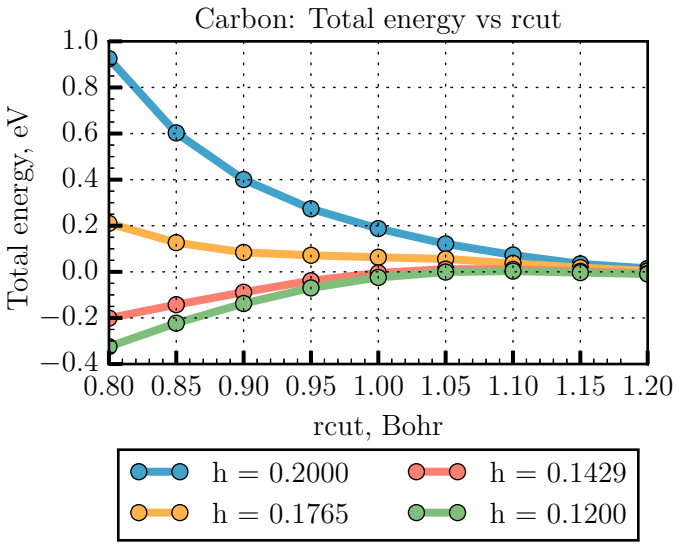


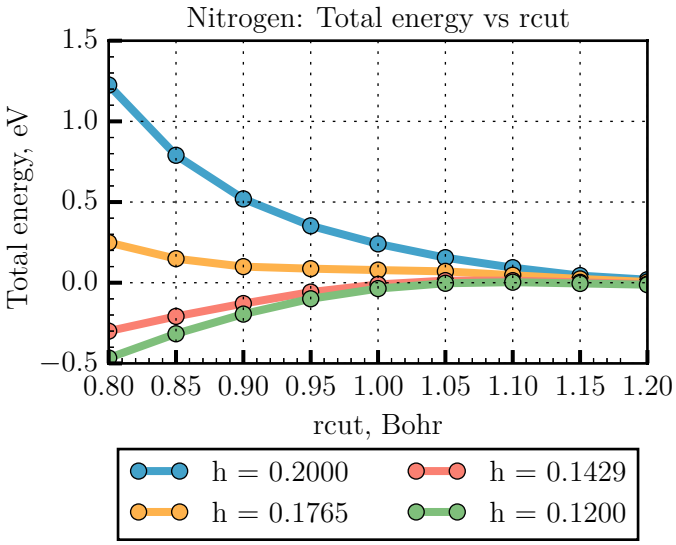


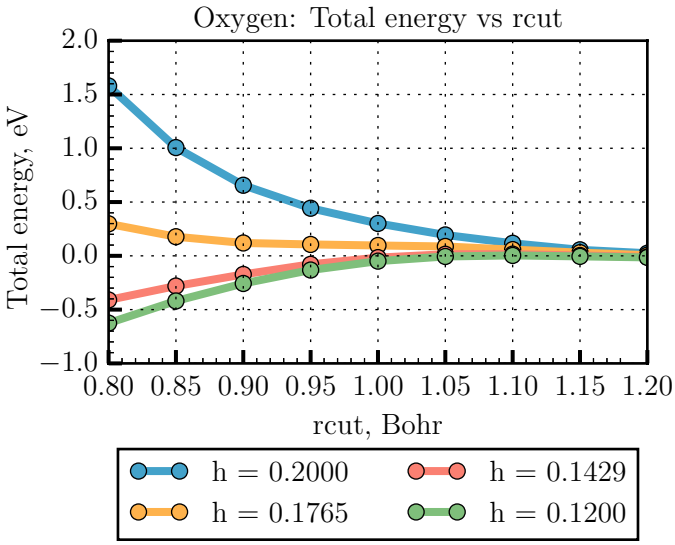









Nitrogen: Total energy vs rcut
Total energy, eV
rcut, Bohr
h = 0.2000
h = 0.1429
h = 0.1765
h = 0.1200


Oxygen: Total energy vs rcut
Total energy, eV
rcut, Bohr
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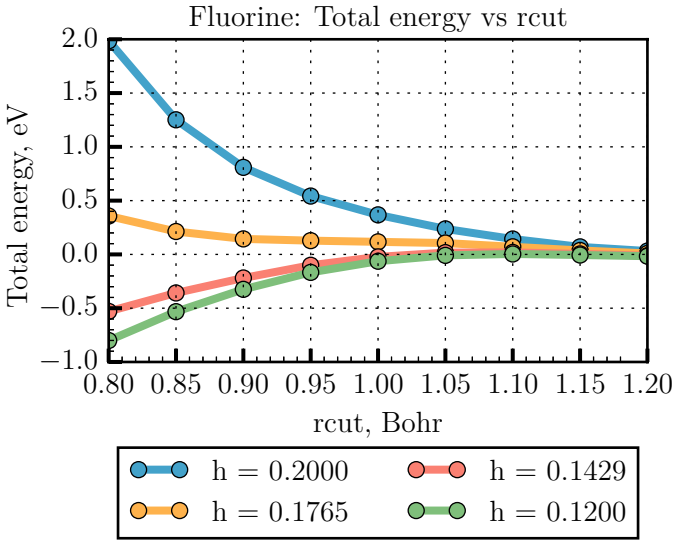
h = 0.1429
h = 0.1765
h = 0.1200


Fluorine: Total energy vs rcut
Total energy, eV
rcut, Bohr
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h = 0.1429
h = 0.1765
h = 0.1200

Calculation time for rcut variation.