Supporting Information for:

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

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Contents:

1. rcut values.
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

Oxygen: Total energy vs rcut

Fluorine: Total energy vs rcut
Calculation time for rcut variation.