# Ultrasoft Pseudopotentials?

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# Overview

I will challenge the "softness" of ultrasoft potentials in two ways

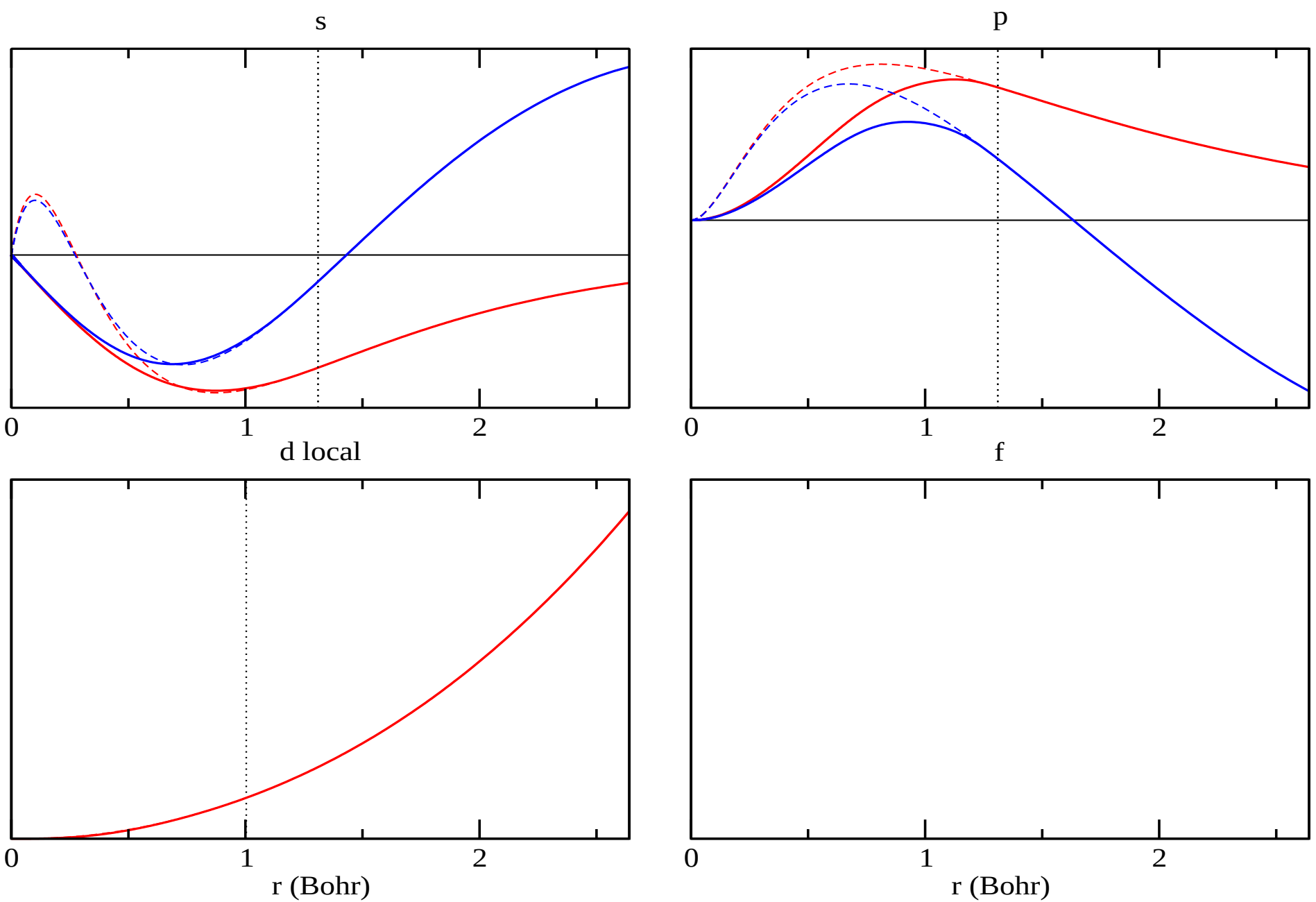
1. The Castep database O_00.usp pseudopotential

2. All electron pseudopotentials

# Ultrasoft pseudopotentials

- Ultrasoft (Vanderbilt) pseudopotentials *can* be soft because norm conservation is not required

- The actual softness depends on the pseudisation scheme chosen

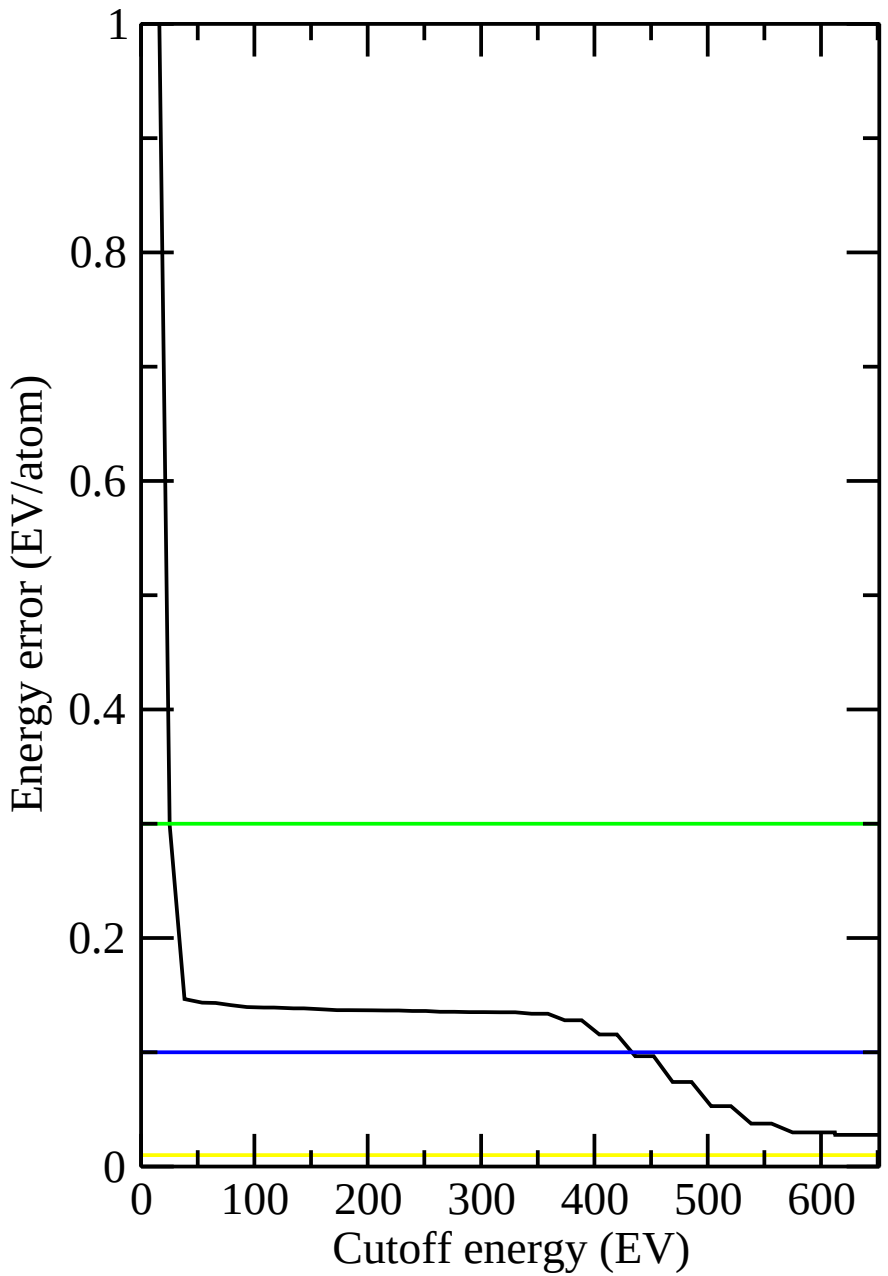

s
p
d local
f
0
1
2
r (Bohr)

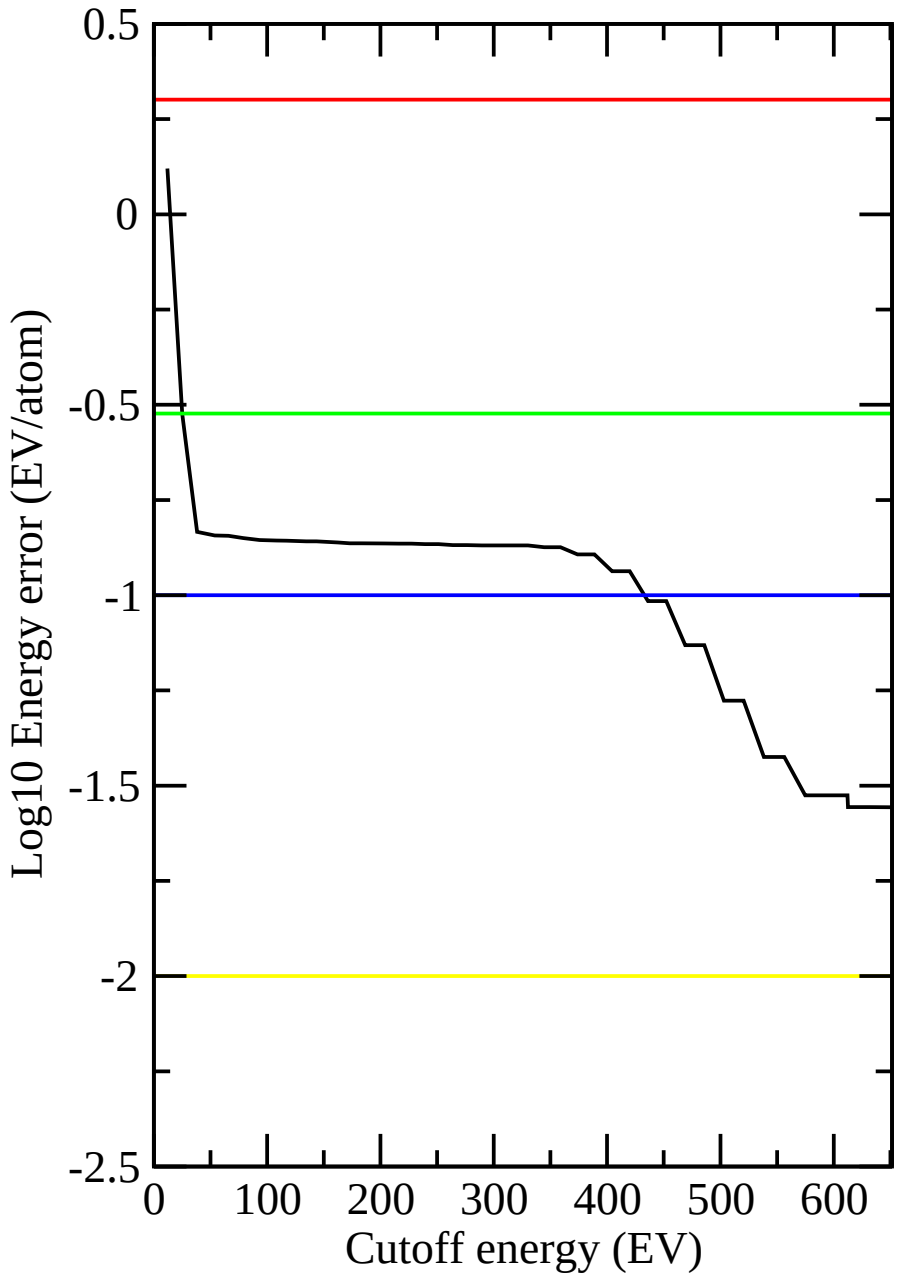
# Pseudisation

- Polynomial fit
- Two bessel function (Kresse)
- Troullier-Martins
- Rappe
- $q_c$ optimisation
- ($q_c$ tuning)

# $Q_c$ Optimisation

Minimise the weight between $q_c$ and $3q_c$


Energy error (EV/atom)
1
0.8
0.6
0.4
0.2
0
0
100
200
300
400
500
600
Cutoff energy (EV)


Log10 Energy error (EV/atom)
0.5
0
-0.5
-1
-1.5
-2
-2.5
0
100
200
300
400
500
600
Cutoff energy (EV)

# The Oxygen Pseudopotential

## O_00.usp

```
START COMMENT
260 COARSE
300 MEDIUM
340 FINE

Ultrasoft potential generated using the setting suggested by
Prof. Vanderbilt's group.
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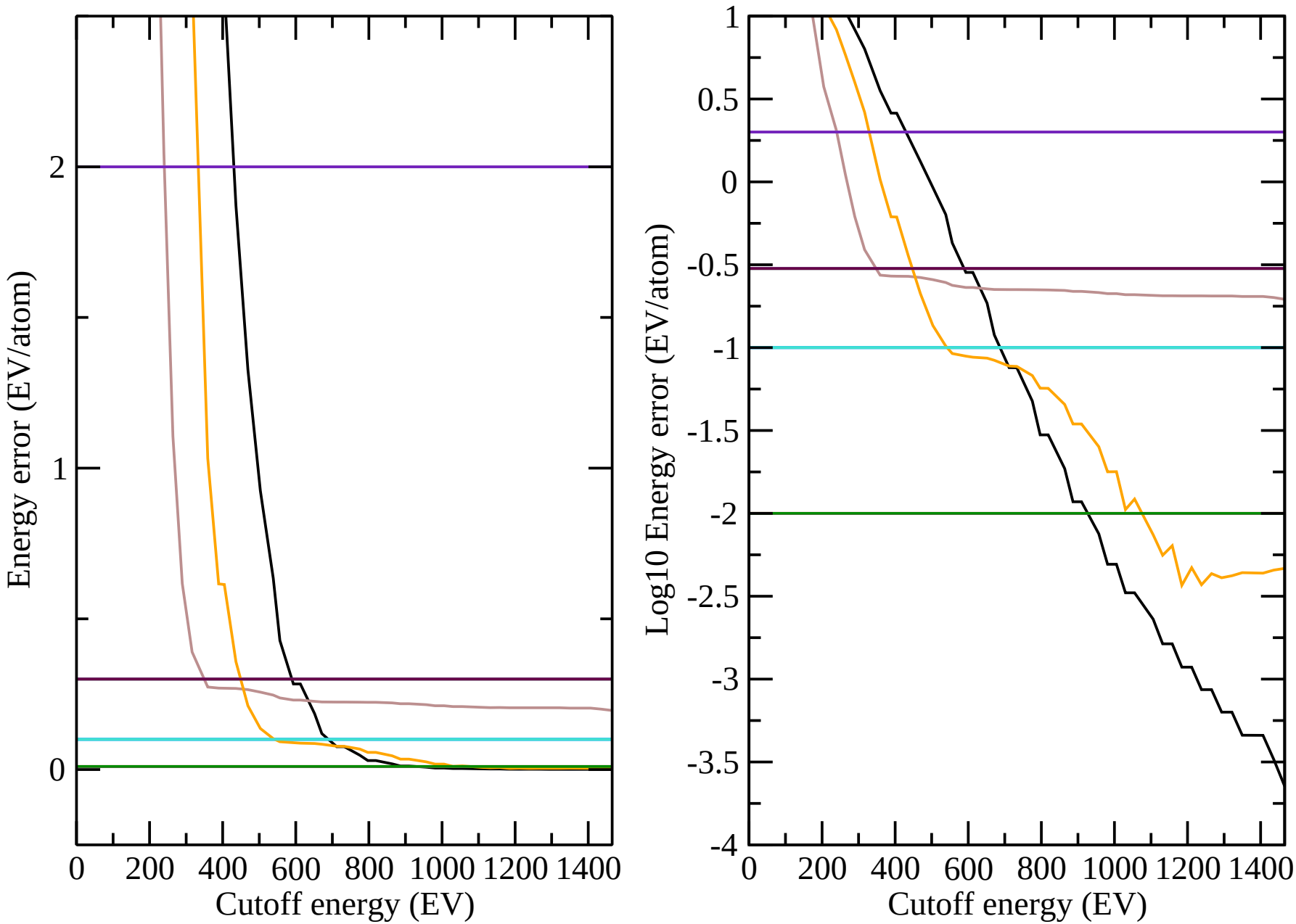
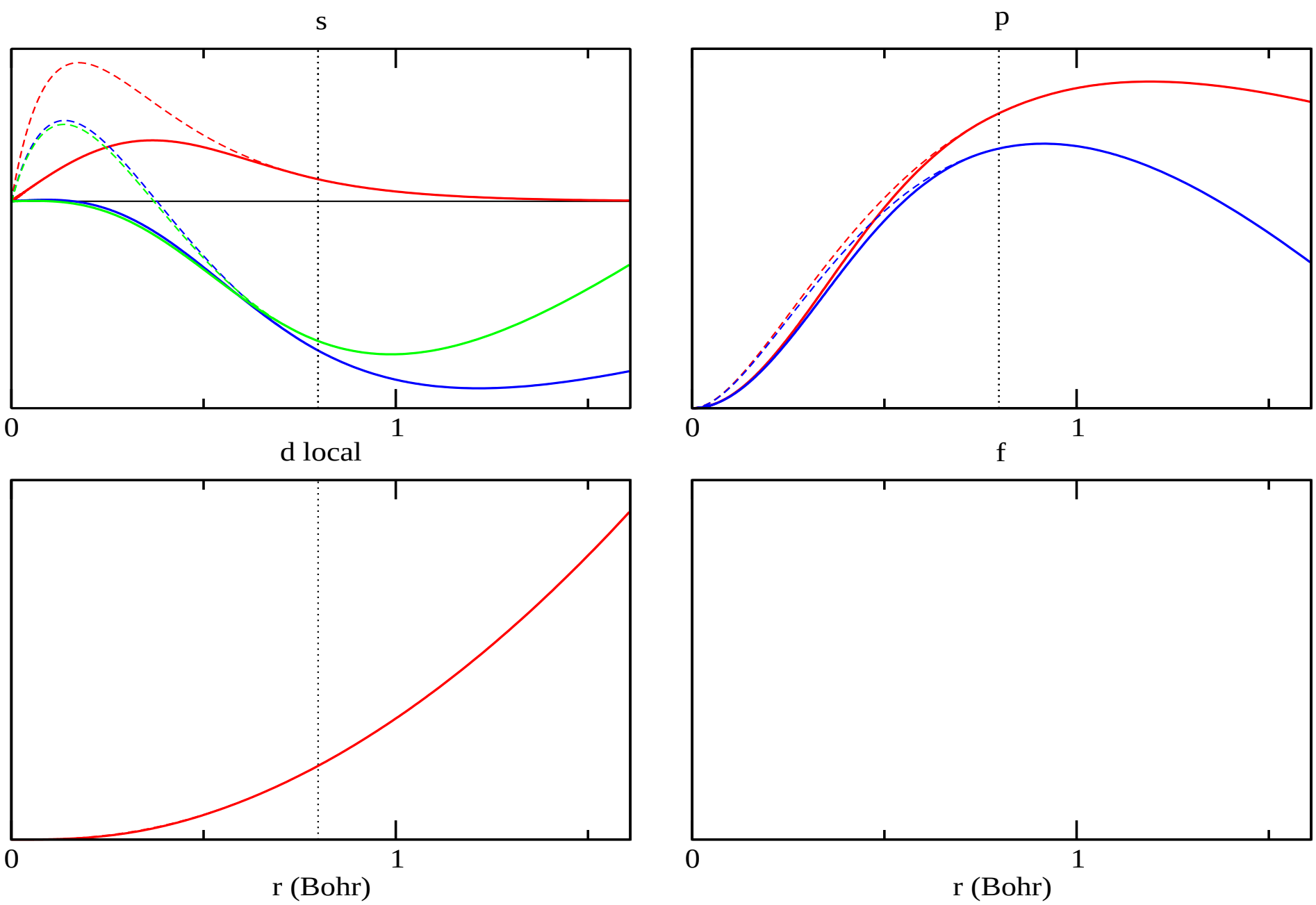
Convergence test

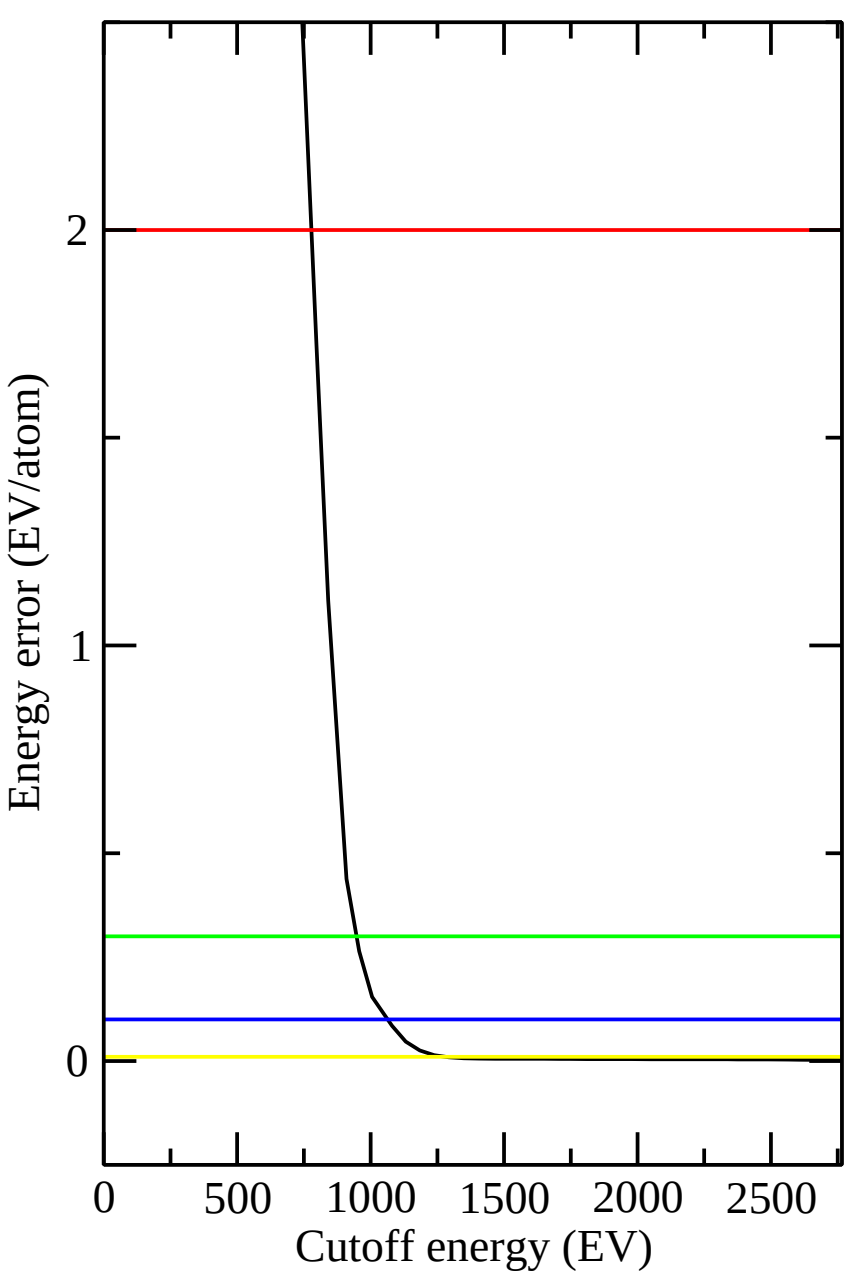
| Ecut (eV) | Etot (eV) | dE (eV/atom) | Force on atom 1 (eV/A) | | |
|---|---|---|---|---|---|
| 260 (COARSE) | -865.339 | 0.995 | -2.18394 | -2.69656 | -2.52689 |
| 280 | -866.293 | 0.518 | -2.56270 | -2.64167 | -2.63499 |
| 300 (MEDIUM) | -866.733 | 0.298 | -2.69282 | -2.74278 | -2.71994 |
| 320 | -867.064 | 0.133 | -2.81231 | -2.83695 | -2.81168 |
| 340 (FINE) | -867.141 | 0.094 | -2.90263 | -2.90146 | -2.95344 |
| 380 (PRECISE) | -867.209 | 0.060 | -2.97010 | -2.96923 | -2.96949 |
| 400 | -867.211 | 0.059 | -2.98485 | -2.98645 | -2.98999 |
| 450 | -867.216 | 0.056 | -3.00329 | -3.00392 | -3.00380 |
| 800 | -867.329 | | -3.04487 | -3.04263 | -3.04365 |

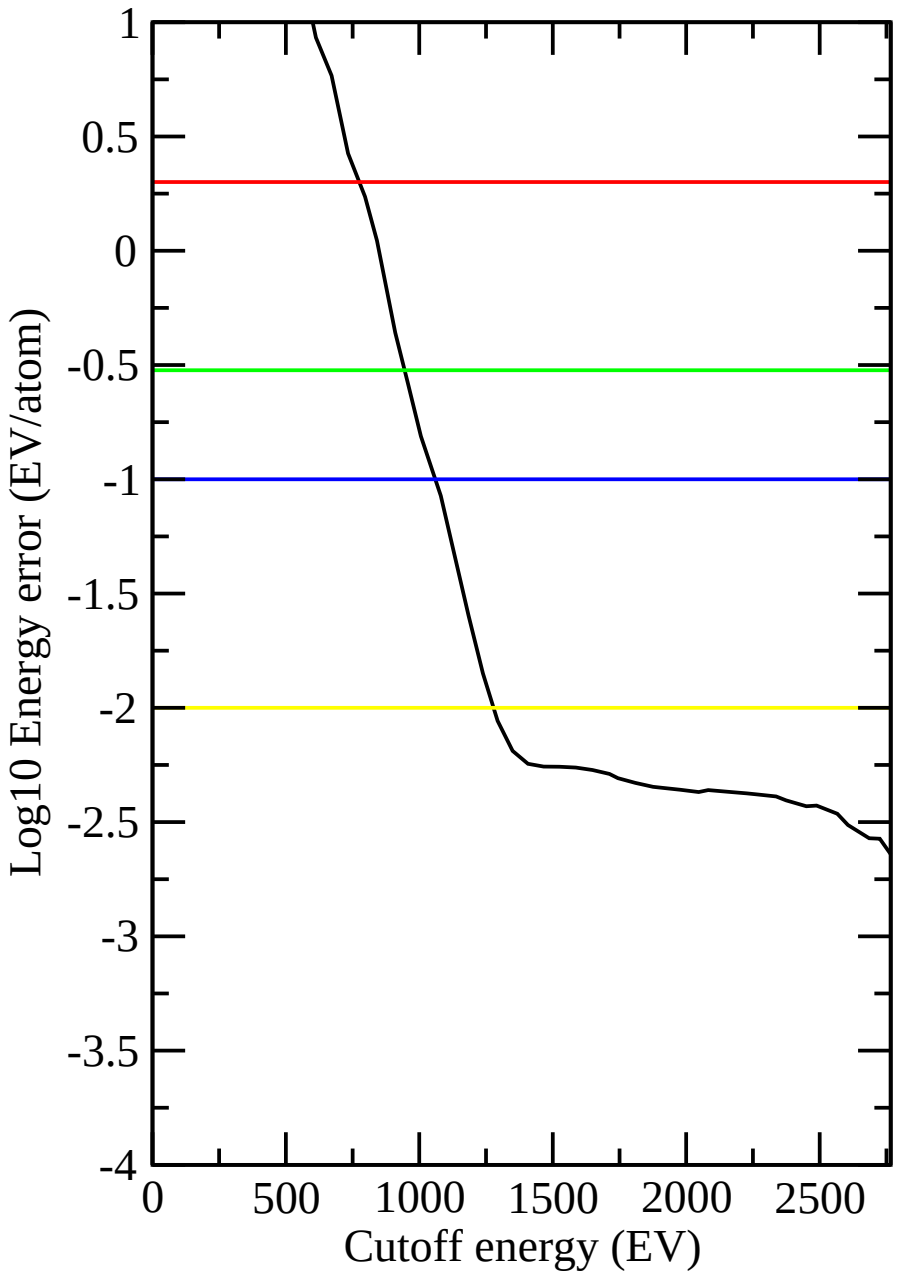

Energy error (EV/atom)
2
1
0
0
200
400
600
800
1000
1200
1400
Cutoff energy (EV)
Log10 Energy error (EV/atom)
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-3
-3.5
-4
0
200
400
600
800
1000
1200
1400
Cutoff energy (EV)

# All electron ultrasoft pseudopotentials

Dropping the norm conservation constraint gives you the freedom to choose core radii, and Vanderbilt's scheme effortlessly makes use of multiple projectors


s
p
0
1
d local
f
0
1
r (Bohr)
0
1
r (Bohr)


Energy error (EV/atom)
2
1
0
0
500
1000
1500
2000
2500
Cutoff energy (EV)


Log10 Energy error (EV/atom)
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-3
-3.5
-4
0
500
1000
1500
2000
2500
Cutoff energy (EV)

# Diamond

| Potential | LDA a/Å | GGA-PBE a/Å |
|---|---|---|
| AE PSP rc = 0.8 | 3.539 | |
| AE PSP rc = 1.2 | 3.538 | 3.579 |
| PSP NLCC rc = 1.2 | 3.533 | 3.571 |
| PSP rc = 1.2 | 3.529 | 3.569 |
| PSP NLCC rc = 1.6 | 3.530 | 3.569 |
| PSP rc = 1.6 | 3.528 | 3.568 |
| C_00.usp rc = 1.4 | 3.525 | 3.566(3.532) |
| | | |
| LAPW | 3.54 | |