

PBE norm conserving Cd pseudopotential for calculations with Quantum ESPRESSO

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A new norm conserving pseudopotential was generated and tested for the Cd atom, for use with Quantum ESPRESSO with the PBE exchange-correlation functional.

I. INTRODUCTION

Ultrasoft pseudopotentials are needed to account for the O $2s,2p$ and Cd $4d$ orbitals with low cutoffs (30 Ry), and these have been used for molecular dynamics and XPS studies of CdTe oxides (Phys. Rev. B 81, 014210 (2010); Phys. Rev. B 79, 014205 (2009)). This is the set (a) in table I, which is completed with a Te norm conserving pseudopotential that was generated for these studies. However, some properties like the dielectric functions and the Raman intensities can be calculated with Quantum ESPRESSO only using norm conserving pseudopotentials. Hence, a norm conserving Cd pseudopotential for PBE calculation is presented here. It has been generated with the Martins-Troulliers algorithm, and together with an available O pseudopotential, completes the set (b) in Table I.

The Cd pseudopotential was generated using the program `ld1`, version 2003-May-27, by P. Giannozzi.

The input file for the generation of the reference state with `ld1` was

```
&input
  atom='Cd',
  config='[Kr] 4d10.0 5s1.0 5p1.0',
  xmin=-9.0, dx=0.02, dft='pbe', file_wavefunctions='cds2p0d10.wfc',
  file_logder='cds2p0d10.logder', emin=-1.0, emax =0.0, rd=2.45
&end
```

Later, the program `trou` was used to generate the pseudopotential, with the following input file (eliminate ! and after for real use).

```
cds2p0d10.wfc ! file of all electron wavefunctions
0.5           ! parameter for nonlinear core correction
0.001        ! radius to cut exchange correlation
5S           ! valence orbital
2.40         ! cutoff radius
5P           ! valence orbital
2.40         ! cutoff radius
4D           ! valence orbital
2.10         ! cutoff radius
             ! blank space
             ! blank space
Cd.pbe-mt.NC ! name of the pseudopotential
```

Then, edit the line

```
'Cd' 12.0 2 0 0 .T. 2 .F.! MT cc0.50 5S1.00 Rc=2.43 5P1.00 Rc=2.43 4D**** Rc=2.11
```

and replace the “2” between “T” and “F” by 1. This defines the local channel of the pseudopotential. With 2, the PWSCF calculation fails, probably due to ghost states. The pseudopotential was converted to UPF format using the program `ncpp2upf` of the Quantum ESPRESSO distribution.

TABLE I: Sets of pseudopotentials used in DFT calculations with the PBE functional.

Element	(a) ultrasoft	(b) norm conserving
Cd	Cd.pbe-mt-lloc1.UPF	Cd.pbe-van.UPF
Te	Te.pbe-rrkj.UPF	Te.pbe-rrkj.UPF
O	O.pbe-rrkjus.UPF	O.pbe-mt.UPF

TABLE II: Cutoff study for a crystal of $\text{Cd}_2\text{Te}_2\text{O}_7$ (Weil, Solid State Science **6**, 29 (2004)). The unit cell contains 44 atoms.

ecutwfc(Ry)	ecutdens(Ry)	Total E(Ry)	Pressure (kbar)	Total Force (Ry/bohr)
60	240	-1928.46202414	28.1233	0.273657
70	280	-1928.78334712	106.34	0.269912
75	300	-1928.81939591	118.727	0.269585
80	320	-1928.83131084	123.697	0.269528
85	340	-1928.83530978	124.967	0.269364
90	360	-1928.83817194	124.4	0.269496
95	380	-1928.84256020	123.163	0.269715
100	400	-1928.84900733	122.013	0.269608
120	480	-1928.87634120	123.687	0.269043
140	560	-1928.87983631	125.597	0.269086
150	600	-1928.88052070	124.917	0.269116
80.0	320	-1928.83131084	123.697	0.269528
80.0	280	-1928.82743345	122.257	0.269845
80.0	240	-1928.82481115	123.647	0.270142
80.0	200	-1928.83214747	124.637	0.268145
80.0	180	-1928.83386289	124.15	0.267563

For these pseudopotentials, a wavefunction cutoff of 80 Ry can be safely used, with a charge density cutoff of 180 Ry. See Table II for the convergence study. Note that a charge density cutoff of four times the wfc cutoff is needed to account for the charge density and the wavefunctions with the same accuracy. However, for density cutoffs of 180 or 320 Ry the total energy difference is 0.035 eV for the 44-atoms unit cell, i.e. 0.78 meV/atom. The pressure difference is 0.45 kbar, and the force difference is 0.001 eV/Å. The DOS calculated using 320 and 180 Ry are practically undistinguishable.

For the same crystal, the Figure 1 shows the density of states calculated with both sets of pseudopotentials. Both DOS are practically equal, the only noticeable, although marginal, difference is a small red shift (~ 0.3 eV) of the band associated with the Cd $4d$ levels. This difference seems to be an effect of difference in Vanderbilt and Martin-Troulliers pseudopotential generation algorithms. I have tested that this shifts is stable against small variations of the MT pseudopotentials building parameters: cutoff radii, the reference state, and the inclusion of the non linear core correction, as well as plane wave cutoffs. These test calculations were done for the CdO rocksalt structure.

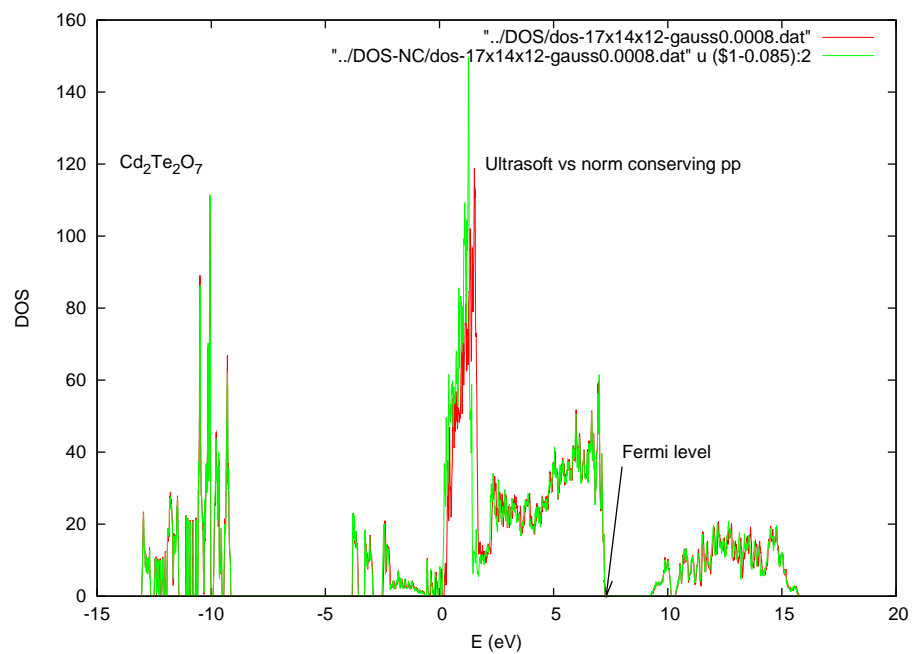


FIG. 1: Density of states of the $\text{Cd}_2\text{Te}_2\text{O}_7$ crystal calculated using both sets of pseudopotentials.