

feedback

on the

small group project

about

“reporting reproducible DFT results”

SMALL - GROUP PROJ

3-4 max

1 Mohaddese Aliveza + Saraz	2 +Fechtakkord JOVAN PRAVEEN
3 SANGESTA ANTARA + SAUANY VIVER	4 + ANIMA PRANJAL Maikus Pedro
5 Abhishek Vikram Rajev + MUNAVAR	6 + Anita Dhanshree Tumantsereg
7 + RITA BAPTISTE FLORIAN Namsrai	8 Saleem Ayaz Khan + Sodkhoo YOUNES

ZWART - KONINKRIJ

9 Abbas Alay + Waqas	10 + Jahub MARCO GIOVANNI FRANCESCO
11 Habib Younes + Mohammad	12
13	14
15	16

Do you think another group will be able to reproduce your results when reading the 'paper' you have submitted ?

1

2

3

4

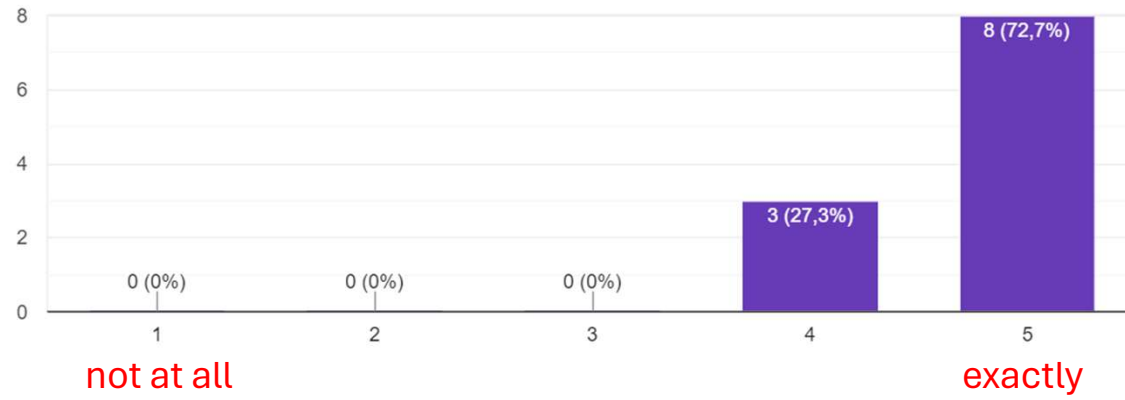
5



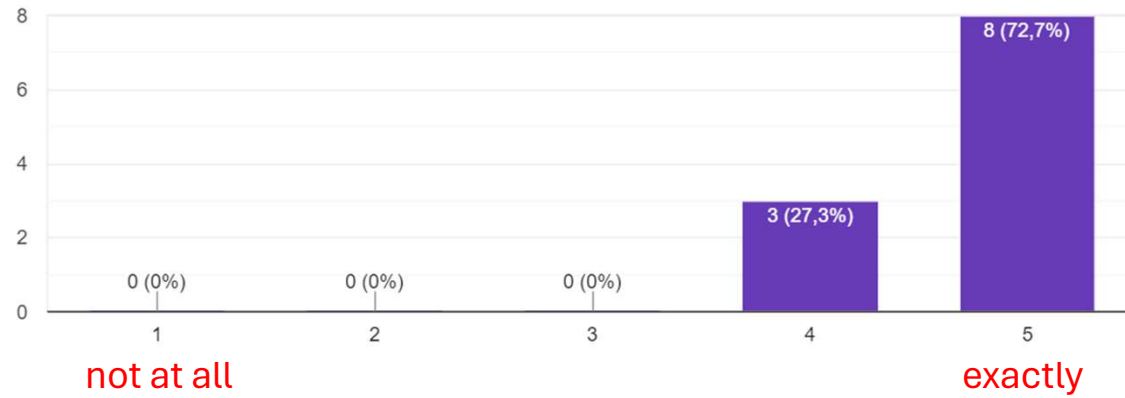
not at all

exactly

Do you think another group will be able to reproduce your results when reading the 'paper' you have submitted ?

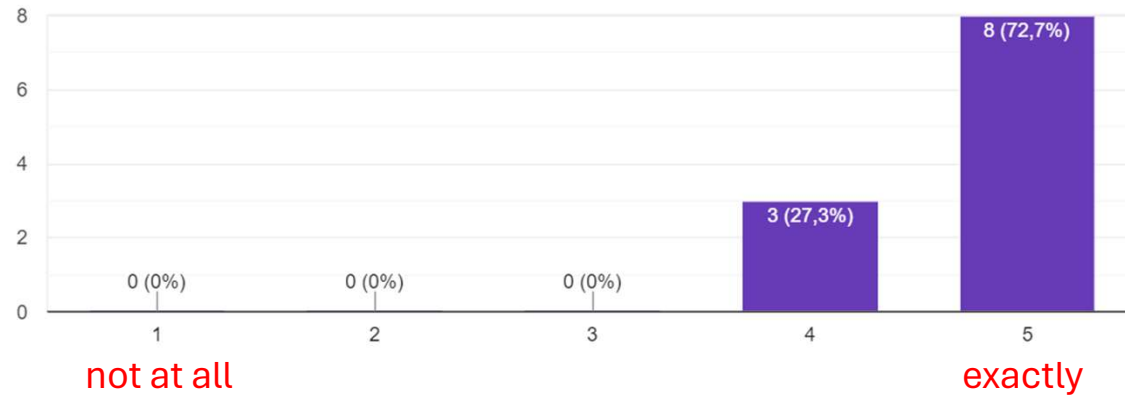


Do you think another group will be able to reproduce your results when reading the 'paper' you have submitted ?

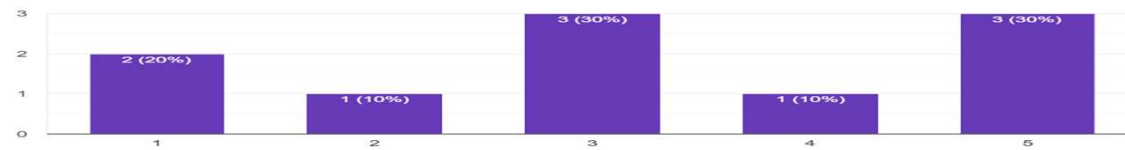


Globally spoken, to what extent do you feel you were successful in reproducing the results that were mentioned in the report you have been given ?

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Globally spoken, to what extent do you feel you were successful in reproducing the results that were mentioned in the report you have been given ?



About round 2: we cannot access the depository any more, and there is not enough information in the report of the other group to generate the structure. Hence we are not able to reproduce these results.



Computational Methods

All the spin polarized DFT calculations were performed on the WIEN2k software package (version 23.1)[1,2], which is based on the full-potential (linearized) augmented plane-wave (LAPW) and local orbitals (lo) method. The exchange correlation energy in the calculation was described by PBE [3] within the GGA formalism. All the calculations were performed on the unit cell of cubic spinel Cr₂CoO₄ (space group #227) [4]. The RMT sphere radii for Cr, Co and O are set to 1.97, 1.99, and 1.71 a.u., respectively. The RKmax value of 5.9 is given and the separation energy of -6 Ry is used for the core-valence electron separation. All the ground state properties were calculated using a 10x10x10 k-mesh resulting in 1000k points (47 k-points in the IBZ). The energy convergence criterion was set to 10⁻⁴ Ry for the SCF cycle.

Results

The total energy of the unit cell of Cr₂CoO₄ is calculated as -15185.33585213 Ry. The global band gap value obtained using the employed PBE functional is 0.177 eV. The total magnetic moment of the cell is 18.0 μB. Magnetic moments on the Cr and Co atoms were found to be 2.65 and 2.71 μB, respectively, while the moment on the O atom is negligible.

References

1. P. Blaha, K. Schwarz, F. Tran, R. Laskowski, G.K.H. Madsen and L.D. Marks, J. Chem. Phys. 152, 074101 (2020)
2. Blaha, P., Schwarz, K., Madsen, G. K., Kvasnicka, D. & Luitz J. wien2k. An augmented plane wave+ local orbitals program for calculating crystal properties, 60 (2001) ISBN 3-9501031-1-2
3. Perdew, J. P., Burke, K. & Ernzerhof, M. Generalized gradient approximation made simple. Phys. Rev. Lett. 77(18), 3865 (1996).
4. <http://wien2k.at/Deposition/Cr2CoO4.cif>

Computational Methods

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References

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3. Perdew, J. P., Burke, K. & Ernzerhof, M. Generalized gradient approximation made simple. Phys. Rev. Lett. 77(18), 3865 (1996).
4. <http://wien2k.at/Depository/Cr2CoO4.cif> alternative link :
<http://wien2k.at/Depository/1Cr2CoO4.cif>

make your final cif files accessible in your publications :

- add them as supplementary info
- deposit them in dedicated databases (COD, ICSD, ...)
- (share them via your website or github or ...)

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or give the full specification of your crystal :

- space group (and setting, if needed)
- all cell parameters (out of 6) that are undetermined by the space group
- names of the wyckoff positions + values of free coordinates

➔ mainly useful for small cells with quite some symmetry

KVF₃ (example)

```
_symmetry_space_group_name_H-M    Pm-3m
_cell_length_a      4.12936034
_cell_length_b      4.12936034
_cell_length_c      4.12936034
_cell_angle_alpha   90.00000000
_cell_angle_beta    90.00000000
_cell_angle_gamma   90.00000000
_symmetry_Int_Tables_number      221
```

```
K+  K0  1  0.00000000  0.00000000  0.00000000  1
V2+ V1  1  0.50000000  0.50000000  0.50000000  1
F-  F2  3  0.00000000  0.50000000  0.50000000  1
```

useful tool : <https://stokes.byu.edu/iso/findsym.php>

KVF₃ (example)

```
_cell_length_a      4.1293603000  
_cell_length_b      4.1293603000  
_cell_length_c      4.1293603000  
_cell_angle_alpha   90.0000000000  
_cell_angle_beta    90.0000000000  
_cell_angle_gamma   90.0000000000  
_cell_volume        70.4122681731
```

```
_symmetry_space_group_name_H-M "P 4/m -3 2/m"  
_symmetry_Int_Tables_number 221  
_space_group.reference_setting '221:-P 4 2 3'
```

```
K+1  K+    1 a  0.00000  0.00000  0.00000  1.00000  0,0,0  
V2+1 V2+   1 b  0.50000  0.50000  0.50000  1.00000  0,0,0  
F-1  F-    3 c  0.00000  0.50000  0.50000  1.00000  0,0,0
```

“KVF₃ has space group 221, with lattice parameter $a=4.1293603$ Å. K occupies the 1a positions, V the 1b and F the 3c. “

GdCl₃ (example)

```
_cell_length_a      7.4583174000  
_cell_length_b      7.4583174000  
_cell_length_c      4.0749048000  
_cell_angle_alpha   90.0000000000  
_cell_angle_beta    90.0000000000  
_cell_angle_gamma   120.0000000000  
_cell_volume        196.3043039843
```

```
_symmetry_space_group_name_H-M "P 63/m"  
_symmetry_Int_Tables_number 176  
_space_group.reference_setting '176:-P 6c'
```

```
Gd3+1 Gd3+      2 c  0.33333  0.66667  0.25000  1.00000  0,0,0  
Cl-1  Cl-       6 h  0.39180  0.30223  0.25000  1.00000  Dx,Dy,0
```

“ GdCl₃ has space group 176, with lattice parameters $a=b=7.4583174$ Å and $c=4.0749048$ Å. Gd occupies the 2c positions, Cl occupies the 6h positions ($x=0.39180$, $y=0.30233$) “

:ENE Initial	:ENE reproduction
-10413.43201084	-10413.4316
-6373.156	-6373.16
-15185.33585213	-15184.97360402
-39111.94	-13037.52
-9742.1970	-9742.22955
-106681.69	106681.69990931
-53157.79265259	-53157.78974572
-50661.52473412	-50661.52644511
-3702.731	-3702.73110561
-106681.69	106681.54330683

:ENE Initial	:ENE reproduction	:GAP initial	:GAP reproduction	:MMTOT initial	:MMTOT reproduction
-10413.43201084	-10413.4316	0.97	1.116	12.0004	12
-6373.156	-6373.16	0.37	0.38	5.999	6.000
-15185.33585213	-15184.97360402	0.177	0	18.0	0
-39111.94	-13037.52	0	0.468	0	3.00158
-9742.1970	-9742.22955	1.698	1.699	5.99983	6.00114
-106681.69	106681.69990931	0.33	0.331	36.98	36.95863
-53157.79265259	-53157.78974572	2.594	2.589	13.99995	14.00198
-50661.52473412	-50661.52644511	2.172	2.183	14.000023	13.99931
-3702.731	-3702.73110561	0.846	0.846	3.000	3.00002
-106681.69	106681.54330683	0.33	1.795	36.98	20.9998

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-9742.1970				5.99983	6.00114
-106681.69	106681.54330683			36.98	36.95863
-53157.79265259	-53157.79265259			13.99995	14.00198
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**Factor 3 (hex/rhom).
Plus other problems.**

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-39111.94	-13037.52	0	0.468	0	3.00158
-9742.1970	-9742.22955	1.698	1.699	5.99983	6.00114
-10668					1.95863
-53157.79265259	-53157.78974572	2.594	2.589	13.99995	14.00198
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Totally different magnetic solution.

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Computational methods

DFT-calculations were performed with the WIEN2k code and the full-potential augmented plane wave plus local orbitals method. All calculations were performed spin-polarized with the PBE-GGA (generalized gradient approximation) functional. The MgCr_2O_4 unit cell was generated with Fd-3m symmetry group and a lattice parameter equal to 8.36 Å. For the definition of the Muffin-Tin potential, the RMTs were set to: 1.86 Å for Mg; 1.97 Å for Cr; and 1.78 Å for O. The electronic density convergence was achieved by testing various values of the k-mesh (9x9x9, 10x10x10 and 11x11x11) and $R_{\text{MT}}^{\text{min}}K_{\text{max}}$ (5, 6 and 7). The best balance between accuracy and efficiency was achieved for a 10x10x10 k-mesh and a $R_{\text{MT}}^{\text{min}}K_{\text{max}}$ of 6.

Perhaps they guessed the free coordinates of oxygen, or took it from another source?

Mg2+	Mg0	8	0.00000000	0.00000000	0.50000000	1
Cr3+	Cr1	16	0.12500000	0.12500000	0.12500000	1
O2-	O2	32	0.11356739	0.38643261	0.61356739	1

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METHOD SECTION:

alternative link :

<http://www.wien2k.at/Depository/1CrCl3.cif>

In this work, we aim to study the properties of a novel ferromagnetic material CrCl₃. The source of the structure of the compound has been obtained from <http://www.wien2k.at/Depository/CrCl3.cif> using the wget function in Linux terminal. The structure of the material is rhombohedral (space group:148) as shown in fig 1. Density Functional Theory (DFT) was applied to the structure using the WIEN2K software [1] using the generalised gradient approximation (GGA) with Perdew, Burke and Ernzerhof (PBE) [2] potentials. The Muffin Tin Radius (RMT) of Cr and Cl was set at 2.27 a.u. and 2.06 a.u. respectively. The RK_{Max} was set at 7 and L_{max} at 10. We also incorporated the spin polarisation calculations. The k points in the Brillouin Zone was set at 225, resulting in an effective mesh of 6x6x6. Parallel computation was done using 4 local hosts, resulting in one iteration of approximately 35 seconds. The starting lattice parameters were $a=b=5.996 \text{ \AA}$ $c=17.885 \text{ \AA}$.

different -prec, and therefore different HDLOs ?

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The computational setup involved a plane wave basis set with a maximum reciprocal lattice vector (RKmax) of 6.50 and a maximum G-vector (GMAX) of 16.0. A $3 \times 3 \times 3$ k-point mesh without shift, comprising 14 k-points, was utilized for Brillouin zone sampling. The self-consistent field (SCF) convergence was achieved after 13 cycles, with a total energy of -53157.79265259 Ry. The calculated band gap for the up spin and down spin states were found to be 4.535 eV and 2.669 eV, respectively, resulting in a global band gap of 2.594 eV. This disparity arises from the distinct positioning of conduction and valence bands relative to the Fermi level, with a notably flat band around 2.6 eV for the down spin. Specifically, the valence band in the down spin resides below the Fermi level, while its counterpart in the up spin touches the Fermi level. The spin magnetic moment within the cell was determined to be 13.99995, while the magnetic moments associated with different atomic species were evaluated. Notably, the Gd^{3+} ion exhibited a significant magnetic moment of 6.92262, whereas the other ions showed relatively smaller or negligible magnetic moments. These results provide insights into the magnetic properties of $NaGdCl_4$ and contribute to the understanding of its electronic structure.

- (no XC functional mentioned)
- no -prec, even no RMTs → hard to reproduce

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-106681.69	106681.54330683	0.33	1.795	36.98	20.9998

Methodology:

alternative link:

<http://wien2k/Depository/1GdCl3.cif>

Density functional theory (DFT) calculations on GdCl_3 were performed with the Wien2k code (23.1), which is based on the all electron full-potential Augmented-Plane-Wave (APW) method. Starting with the single-crystal structure found from this repository (~~<http://wien2k/Depository/GdCl3.cif>~~), we adopted **spin polarized** scf calculation for calculating the band gap, spin moment of individual atom and the cell at the level of generalized gradient approximation (PBE-GGA). The calculations were initialized with **default settings** within Wien2k except energy cut-off and k-mesh. Here we used the plane wave cutoff parameter **$\text{RK}_{\text{max}} = 7$** for three different total number of K-points ($\text{NUMK} = 700, 324$ and 1100) with atomic spheres of 2.5, 2.38 Bohr for Gd and Cl, respectively.

A script to reproduce the results presented is available on our Gitlab (<https://gitlab.com/ghostjoad/wien2k-gdcl3>).

- Are 'default settings' uniquely defined? (-prec ?)
- Good practice to share workflow scripts (one of the goals of workflow managers)

:ENE Initial	:ENE reproduction	:GAP initial	:GAP reproduction	:MMTOT initial	:MMTOT reproduction
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-6373.156	-6373.16	0.37	0.38	5.999	6.000
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-39111.94	-13037.52	0	0.468	0	3.00158
-9742.1970	-9742.22955	1.698	1.699	5.99983	6.00114
-106681.69	106681.69990931	0.33	0.331	36.98	36.95863
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-3702.731	-3702.73110561	0.846	0.846	3.000	3.00002
-106681.69	106681.54330683	0.33	1.795	36.98	20.9998

Methodology

The calculation for the CoF₂ structure [1] was performed in the framework of density functional theory (DFT) using full-potential augmented plane waves plus local orbital (FP-LAPW+lo), as implemented in WIEN2k code [2]. The exchange-correlation energy of the electrons was calculated in the generalized gradient approximation (GGA) presented by Perdew-Burke-Ernzerhof (PBE) [3]. The valence wave functions inside the muffin-tin spheres were expanded up to $l_{\max} = 10$. The charge density was Fourier expanded up to $G_{\max} = 16$. The potential was expanded inside Muffin-Tin (MT) spheres in combination with spherical harmonic functions and the Brillouin zone for the self-consistent field (scf) calculation was sampled by $8 \times 8 \times 10$ grid k -points, according to the Monkhorst-Pack scheme [4]. The cut-off energy for the separation of valance and core electrons was chosen -6.0 Ry which corresponds to $R_{\text{MT}}K_{\max} = 8.5$, where R_{MT} is the smallest of all atomic sphere radii and K_{\max} determines the truncation of the reciprocal lattice expansion of the wave functions in the interstitial region. The selected R_{MT} for Co and F atoms was 1.910 and 1.730 a.u., respectively. The criterion of energy convergence was set to 10^{-4} Ry per unit cell which led to the total energy of -6373.156 Ry. We also performed spin-polarized calculation to find out the magnetic ordering of the material. The results indicate that this material is a ferromagnetic semiconductor with a direct bandgap of 2.624 (0.370) eV for spin-up (down) and the total spin moment of 5.999 μ_B/cell . Furthermore, the moment of Co (F) atom was obtained as 2.642 (0.128) μ_B .

References

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- Obvious information (not necessarily in this order):
 -) basis set (linearised augmented plane-waves + local orbitals, plane waves, Gaussians, numerical orbitals,...) + **basis set size**
 -) exchange and correlation functional
 -) code used (Wien2K,...)
 -) Core states vs. valence states (see next slides)
 -) k -points (shifted/unshifted)

Methodology

The calculation for the CoF₂ structure [1] was performed in the framework of density functional theory (DFT) using full-potential augmented plane waves plus local orbital (FP-LAPW+lo), as implemented in WIEN2k code [2]. The exchange-correlation energy of the electrons was calculated in the generalized gradient approximation (GGA) presented by Perdew-Burke-Ernzerhof (PBE) [3]. The valence wave functions inside the muffin-tin spheres were expanded up to $l_{\max} = 10$. The charge density was Fourier expanded up to $G_{\max} = 16$. The potential was expanded inside Muffin-Tin (MT) spheres in combination with spherical harmonic functions and the Brillouin zone for the self-consistent field (scf) calculation was sampled by $8 \times 8 \times 10$ grid k -points, according to the Monkhorst-Pack scheme [4]. The cut-off energy for the separation of valence and core electrons was chosen -6.0 Ry which corresponds to $R_{\text{MT}}K_{\max} = 8.5$, where R_{MT} is the smallest of all atomic sphere radii and K_{\max} determines the truncation of the reciprocal lattice expansion of the wave functions in the interstitial region. The selected R_{MT} for Co and F atoms was 1.910 and 1.730 a.u., respectively. The criterion of energy convergence was set to 10^{-4} Ry per unit cell which led to the total energy of -6373.156 Ry. We also performed spin-polarized calculation to find out the magnetic ordering of the material. The results indicate that this material is a ferromagnetic semiconductor with a direct bandgap of 2.624 (0.370) eV for spin-up (down) and the total spin moment of 5.999 μ_B/cell . Furthermore, the moment of Co (F) atom was obtained as 2.642 (0.128) μ_B .

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- Obvious information (not necessarily in this order):
 -) other parameters that regulate precision/convergence (e.g. cutoff energy)
 -) occupation scheme for Kohn-Sham eigenstates (smearing scheme, smearing width)
 -) convergence criteria for the selfconsistent cycle, and in case for relaxation
 -) structure and simulation cell (see next slides)
 - [-) for molecular dynamics: ensemble, thermostat, bariostat, temperature, pressure]

REFERENCES!

Methodology

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report explicitly which states were treated as valence (sometimes it is enough to report the number of valence electrons)

for Wien2K, state also which states were treated as semi-core

for pseudopotential codes, report also kind of pseudopotential, and also database/specific name

Methodology

The calculation for the **CoF₂ structure [1]** was performed in the framework of density functional theory (DFT) using full-potential augmented plane waves plus local orbital (FP-LAPW+lo), as implemented in WIEN2k code [2]. The exchange-correlation energy of the electrons was calculated in the generalized gradient approximation (GGA) presented by Perdew-Burke-Ernzerhof (PBE) [3]. The valence wave functions inside the muffin-tin spheres were expanded up to $l_{\max} = 10$. The charge density was Fourier expanded up to $G_{\max} = 16$. The potential was expanded inside Muffin-Tin (MT) spheres in combination with spherical harmonic functions and the Brillouin zone for the self-consistent field (scf) calculation was sampled by $8 \times 8 \times 10$ grid k -points, according to the Monkhorst-Pack scheme [4]. The cut-off energy for the separation of valence and core electrons was chosen -6.0 Ry which corresponds to $R_{\text{MT}}K_{\max} = 8.5$, where R_{MT} is the smallest of all atomic sphere radii and K_{\max} determines the truncation of the reciprocal lattice expansion of the wave functions in the interstitial region. The selected R_{MT} for Co and F atoms was 1.910 and 1.730 a.u., respectively. The criterion of energy convergence was set to 10^{-4} Ry per unit cell which led to the total energy of -6373.156 Ry. We also performed spin-polarized calculation to find out the magnetic ordering of the material. The results indicate that this material is a ferromagnetic semiconductor with a direct bandgap of 2.624 (0.370) eV for spin-up (down) and the total spin moment of $5.999 \mu_B/\text{cell}$. Furthermore, the moment of Co (F) atom was obtained as 2.642 (0.128) μ_B .

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Also in this case, there should be enough information to identify the structure of crystal/surface/molecule:

one could specify also the ICSD or COD code, space group + Wyckoff sites + all free parameters;

or [.cif](#) file in the supporting information;

gaining ground: put structures, or the whole input files, in public repositories, either on personal spaces ([github](#)) or on public databases (e.g. [Zenodo](#) by CERN)

Methodology

The calculation for the CoF₂ structure [1] was performed in the framework of density functional theory (DFT) using full-potential augmented plane waves plus local orbital (FP-LAPW+lo), as implemented in WIEN2k code [2]. The exchange-correlation energy of the electrons was calculated in the generalized gradient approximation (GGA) presented by Perdew-Burke-Ernzerhof (PBE) [3]. The valence wave functions inside the muffin-tin spheres were expanded up to $l_{\max} = 10$. The charge density was Fourier expanded up to $G_{\max} = 16$. The potential was expanded inside Muffin-Tin (MT) spheres in combination with spherical harmonic functions and the Brillouin zone for the self-consistent field (scf) calculation was sampled by $8 \times 8 \times 10$ grid k -points, according to the Monkhorst-Pack scheme [4]. The cut-off energy for the separation of valence and core electrons was chosen -6.0 Ry which corresponds to $R_{\text{MT}}K_{\text{max}} = 8.5$, where R_{MT} is the smallest of all atomic sphere radii and K_{max} determines the truncation of the reciprocal lattice expansion of the wave functions in the interstitial region. The selected R_{MT} for Co and F atoms was 1.910 and 1.730 a.u., respectively. The criterion of energy convergence was set to 10^{-4} Ry per unit cell which led to the total energy of -6373.156 Ry. We also performed spin-polarized calculation to find out the magnetic ordering of the material. The results indicate that this material is a ferromagnetic semiconductor with a direct bandgap of 2.624 (0.370) eV for spin-up (down) and the total spin moment of 5.999 μ_B/cell . Furthermore, the moment of Co (F) atom was obtained as 2.642 (0.128) μ_B .

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Specific for wien2k:

- ✘ wien2k version 23.2
- ✘ initialization with `-prec 0-3(n)`
defines HDLO basis and several computational parameters:
- ✓ $R_{\min}K_{\max}$ (plane-wave cutoff)
- ✓ RMTs for all atoms
- ✓ GMAX (Fourier series for charge density/potential)
- ✘ FFTfactor (additional factor for XC-potential FFT mesh)
- ✓ ✘ L-vns (max l for $H_{\text{non-spher.}}$) (and also l_{\max})
- ✓ ✘ E-cut (or charge-cut) for core-valence separation, or better an explicit list of core states, semicore (treated with LOs) and valence states. Explicit list for HDLOs (or HELOs)

Methodology

The calculation for the CoF₂ structure [1] was performed in the framework of density functional theory (DFT) using full-potential augmented plane waves plus local orbital (FP-LAPW+lo), as implemented in WIEN2k code [2]. The exchange-correlation energy of the electrons was calculated in the generalized gradient approximation (GGA) presented by Perdew-Burke-Ernzerhof (PBE) [3]. The valence wave functions inside the muffin-tin spheres were expanded up to $l_{\max} = 10$. The charge density was Fourier expanded up to $G_{\max} = 16$. The potential was expanded inside Muffin-Tin (MT) spheres in combination with spherical harmonic functions and the Brillouin zone for the self-consistent field (scf) calculation was sampled by $8 \times 8 \times 10$ grid k -points, according to the Monkhorst-Pack scheme [4]. The cut-off energy for the separation of valence and core electrons was chosen -6.0 Ry which corresponds to $R_{\text{MT}}K_{\max} = 8.5$, where R_{MT} is the smallest of all atomic sphere radii and K_{\max} determines the truncation of the reciprocal lattice expansion of the wave functions in the interstitial region. The selected R_{MT} for Co and F atoms was 1.910 and 1.730 a.u., respectively. The criterion of energy convergence was set to 10^{-4} Ry per unit cell which led to the total energy of -6373.156 Ry. We also performed spin-polarized calculation to find out the magnetic ordering of the material. The results indicate that this material is a ferromagnetic semiconductor with a direct bandgap of 2.624 (0.370) eV for spin-up (down) and the total spin moment of 5.999 μ_B/cell . Furthermore, the moment of Co (F) atom was obtained as 2.642 (0.128) μ_B .

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The methods section: more details on the Hamiltonian

For a simple Kohn-Sham Hamiltonian, specification of the exchange and correlation functional is sufficient

However, more sophisticated Hamiltonians require further specifications:

-) Hubbard U correction comes in different flavours
-) spin-orbit coupling (e.g. mention scalar-relativistic)
-) hybrid functionals
-) van der Waals potentials/functionals
-) ...

For example, details of how selfconsistency is reached (preconditioning, mixing) affect speed of convergence, but 'usually' not the final result.

However, there might be difficult cases where this information is important to reach selfconsistency at all (magnetic systems...)

conclusion

reporting about DFT (WIEN2k) calculations such that they are reproducible is hard work



conclusion

reporting about DFT (WIEN2k) calculations
such that they are reproducible is hard work

but definitely possible

(you have inspiration and a check-list now)