Name Surname Data

AMM Lab 1

Choose a simple semiconductor or insulator containing transition metal. The transition metal must have at least two *d* (two *f*) and nine or less than nine *d* (thirteen or less than thirteen *f*) electrons after oxidation. Pay attention to the magnetic configuration. Provide a link to the input and output files.

1. Introduction

Description of material's properties and possible application in real life. (1.5 page)
Mention Materials project ID.
Mention symmetry space group.
Give a description of the crystalline structure and Brillouin zone

2. Theory

Description of used theoretical approach. (1/2 page). Mention name of pseudopotentials that you have used, and corresponding URL with download parameters. By default, PS Library, PAW PBE http://pseudopotentials.quantum-espresso.org/upf_files/Ga.pbe-dn-kjpaw_psl.1.0.0.UPF for the computation of total energy, optimization of geometry, while for the specific computation of TB09 band gaps, use http://www.pseudo-dojo.org/ NC SR, PBE, Accuracy standard, Format UPF, and perform non-self-consistent calculations at the previously determined lattice parameters and atomic positions. Definition of the *U* in DFT+*U:* How *U* value is connected with the total energy? What is projected DOS?

3. Results

Description of obtained results (8 pages) Give both: graphical representations (see examples in the next pages) and tables with raw data for sections A-D. For sections E-F provide a band structure figure. One page for each of the following sections.

A. Total energy as a function of planewave cut-off energy
B. Total energy as a function of wavevector sampling
C. Cell parameters as a function of planewave cut-off energy
D. Cell parameters as a function of wavevector sampling
E. . Electronic DOS and band structure with the GGA-PBE exchange-correlation functional
F. Electronic DOS and band structure with the TB09 exchange-correlation functional
G. Cell parameters as a function of *U*
H. Projected electronic DOS for various *U*

4. Discussion

Which values of planewave cut-off energy and wavevector sampling gives accurate numerical values for the total energy?
Same question for the geometrical parameters?
With this cut-off energy and wavevector sampling which values do you get for the lattice parameters and atomic positions?
Compare with the Materials Project data (both obtained from VASP calculation using GGA-PBE -main MP page.

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How does the electronic structure changes with different *U*? Which *U* value is the best choice for your material? How can you decide it? What is the physical meaning of *U* in DFT+*U*? Compare possibly with other bibliographical information (1 page)

5. Conclusions

Summarize what you have obtained and why it could be important for future applications. (1/2 page)

6. References

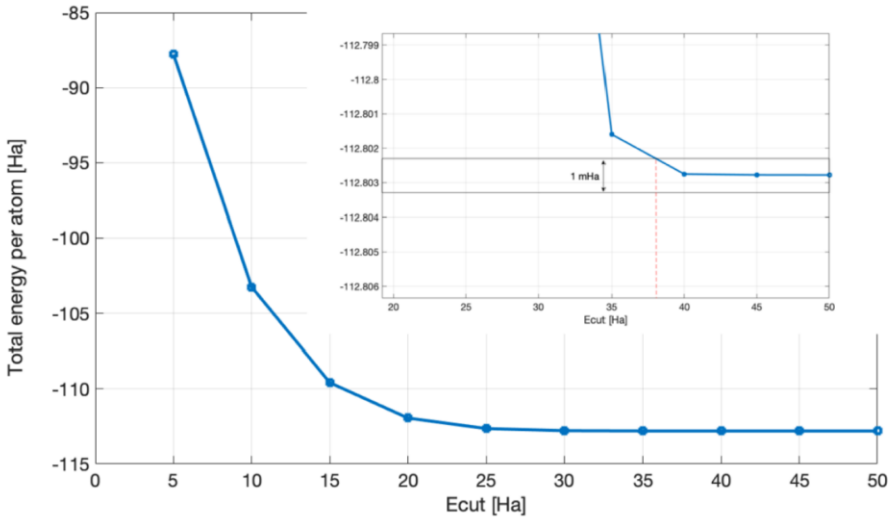
All your work must be supported by references and the format must be used the same of American Chemical Society (Looks in ACS journals: JACS).

The students must use the format of this template font Times New Roman 12 pt for title section and 10 pt for text session. Different formats and short or longer reports than requested will be not evaluated

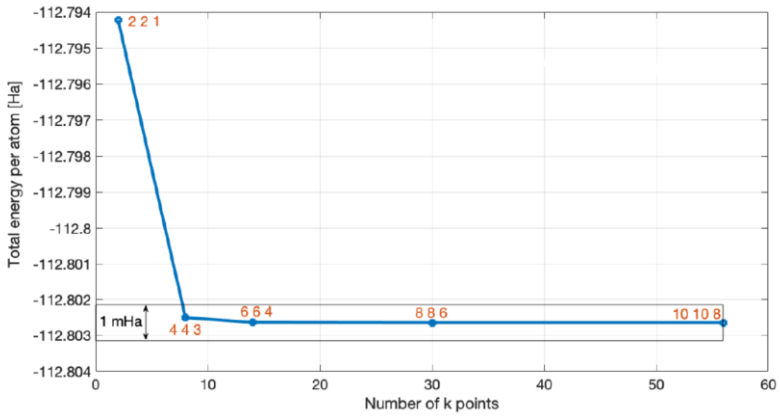
Examples of figures for section 3.

A-F obtained for ZnO, a crystal belonging to the hexagonal crystallographic system, with lattice parameters a=b perpendicular to the hexagonal axis and c along the hexagonal axis. The raw data must also be provided, in the form of tables for sections A-D.

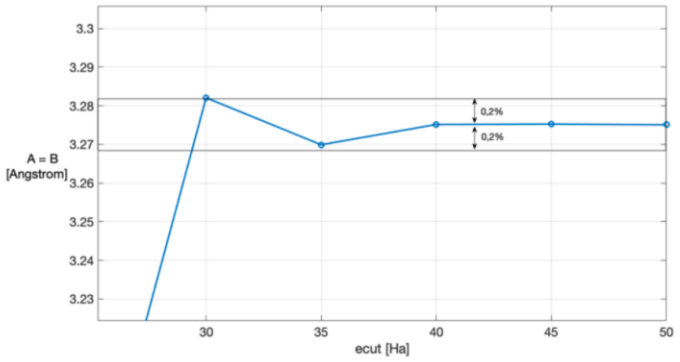
A. Total energy as a function of planewave cut-off energy

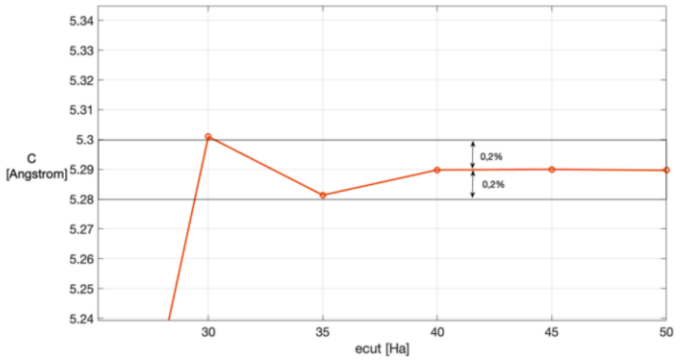


B. Total energy as a function of wavevector sampling

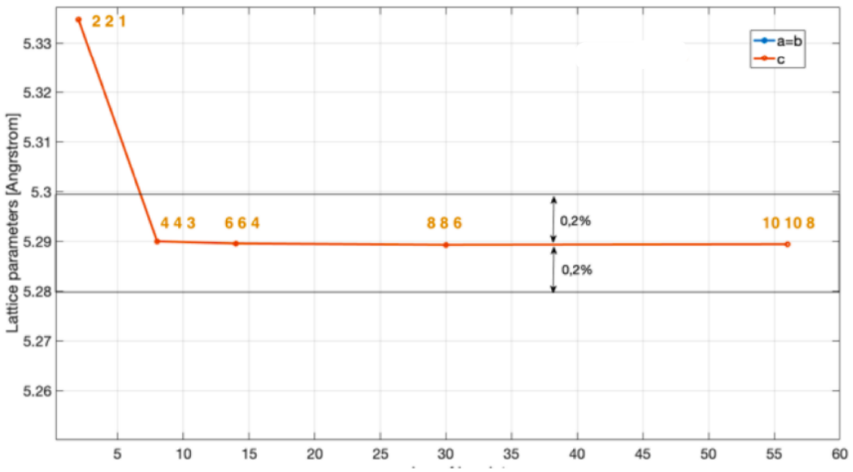


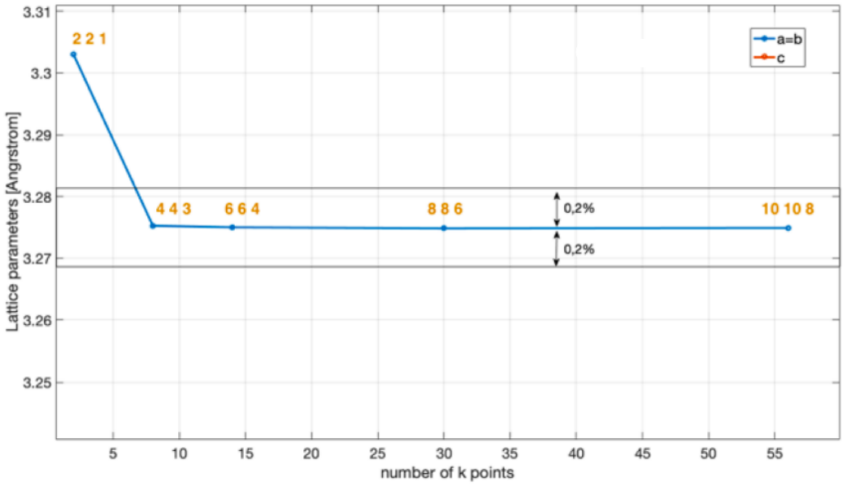
C. Cell parameters as a function of planewave cut-off energy





D. Cell parameters as a function of wavevector sampling





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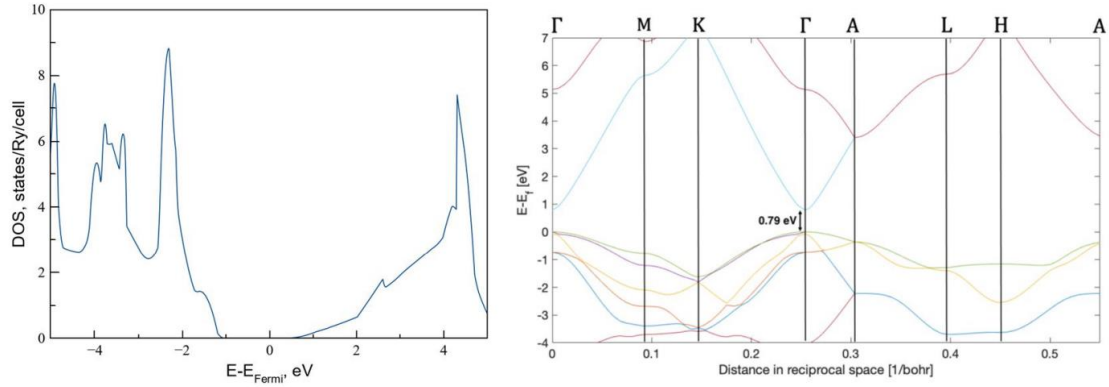
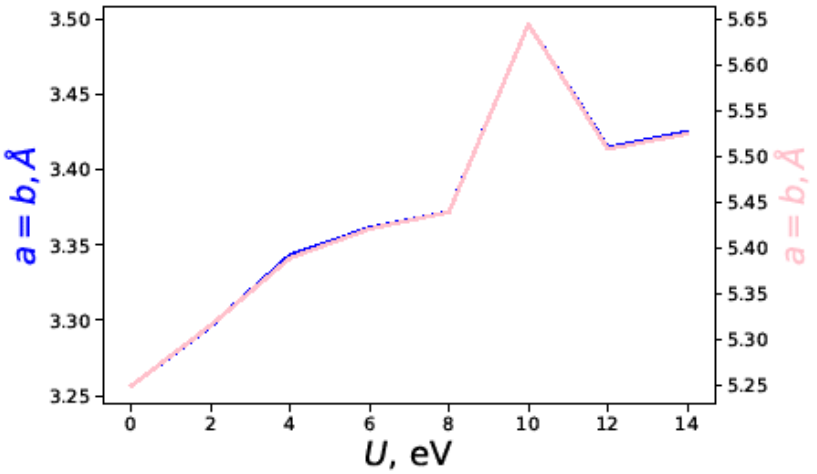
E. Electronic DOS

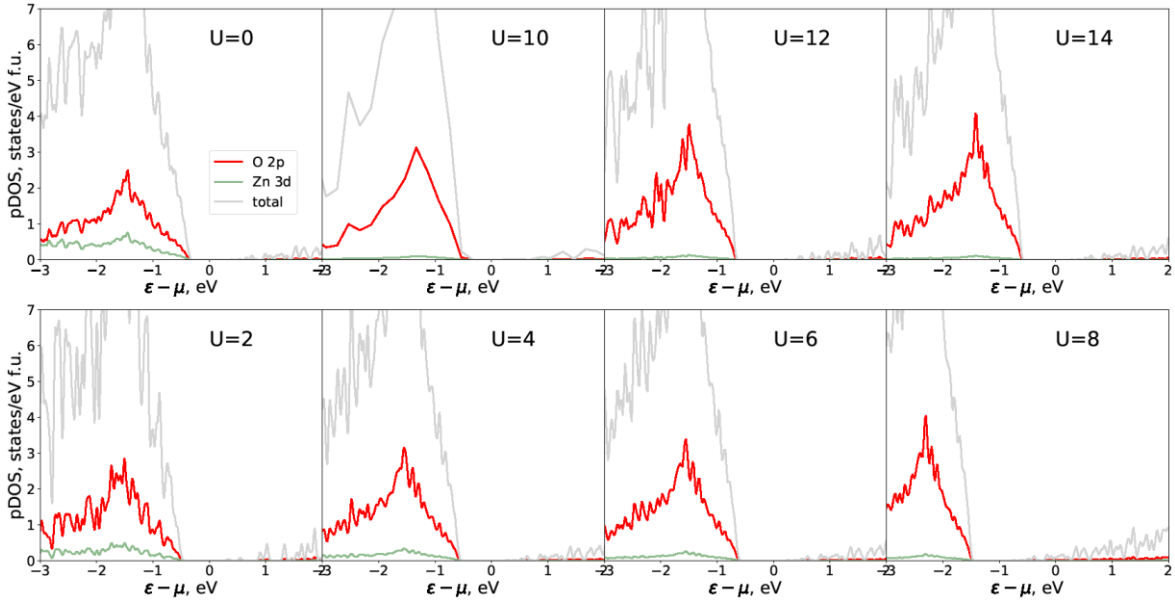
F. and band structure



G. Cell parameters as a function of U



H. Densities of states for various U



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