STUDY OF ELECTRONIC PROPERTIES OF INSULATOR XX

I. Introduction

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

II. Theory

Description of theoretical approach used. (1/2 page)
Mention name of pseudopotentials that you have used, and corresponding URL with download parameters. By default, http://www.pseudo-dojo.org with PAW JTH v1.0, XC PBE, Accuracy Standard, Format psp8 for the computation of total energy, optimization of geometry,
while for the specific computation of TB09 band gaps, use http://nninc.cnf.cornell.edu/dd_search.php?frmxcprox=&frmxctype=&frmspclass=HGH , and perform non-self-consistent calculations at the previously determined lattice parameters and atomic positions.

III. Results

Description of obtained results (6 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, as well as a table with eigenenergies at selected wavevectors, only for the highest occupied band and the lowest occupied band.
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 band structure with the GGA-PBE exchange-correlation functional
F. Electronic band structure with the TB09 exchange-correlation functional

IV. 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 these 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- and from ABINIT using GGA-PBEsol from the Abinit DDB). Compare possibly with other bibliographical information (1 page)

V. Conclusion

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

VI. References

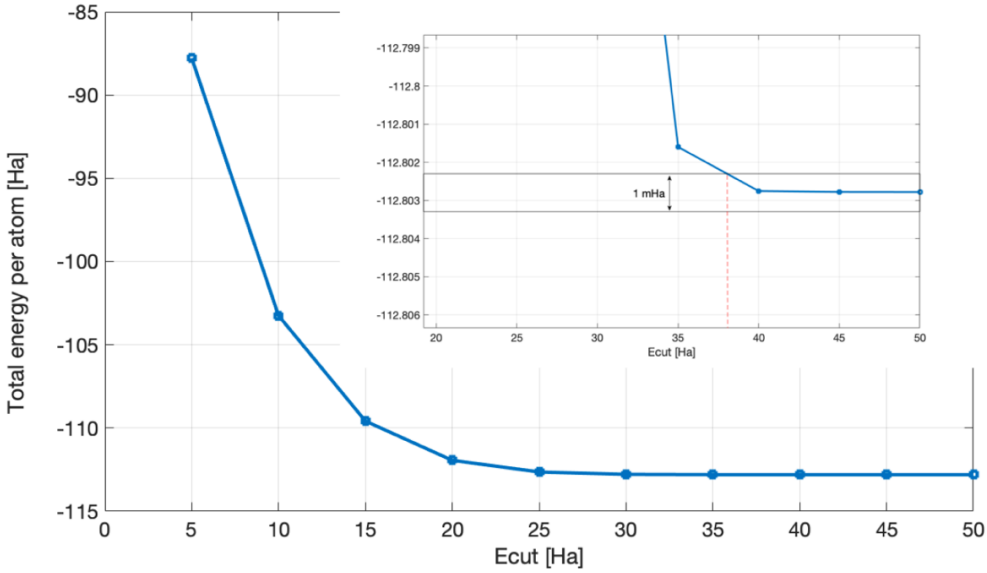
All your work must be supported by references and the format must be used the same of American Chemical Society (Looks in ACS journals: JACS).

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.

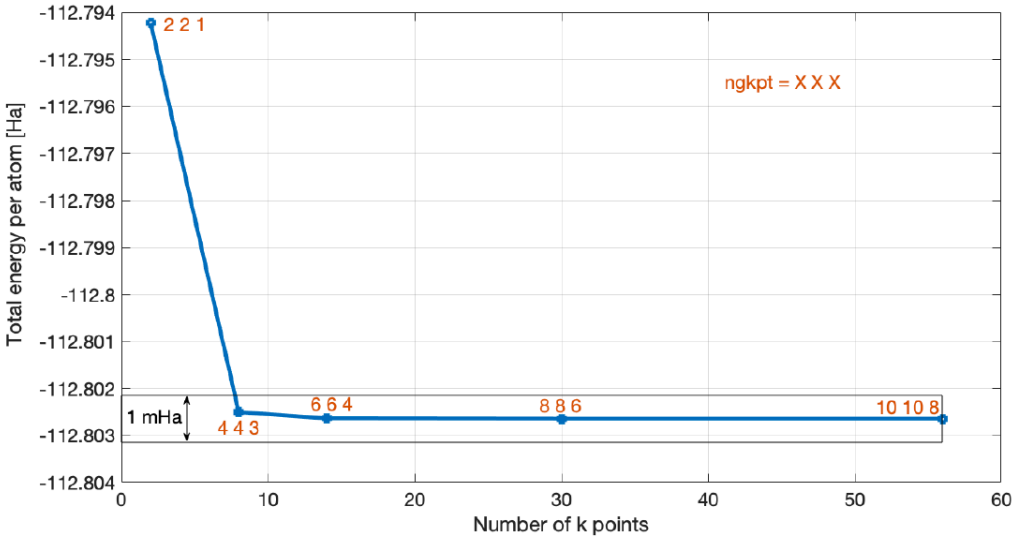
Name Surname AMM Lab 1 Date

Examples of figures for sections III.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. For sections E-F provide a table with eigenenergies at selected wavevectors, only for the highest occupied band and the lowest occupied band. One page for one section .

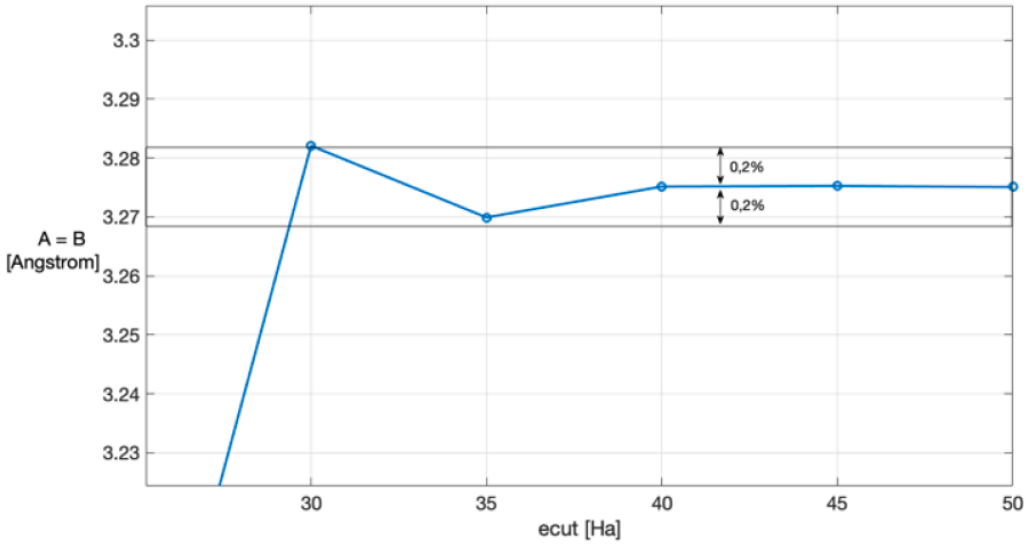
A. Total energy as a function of planewave cut-off energy

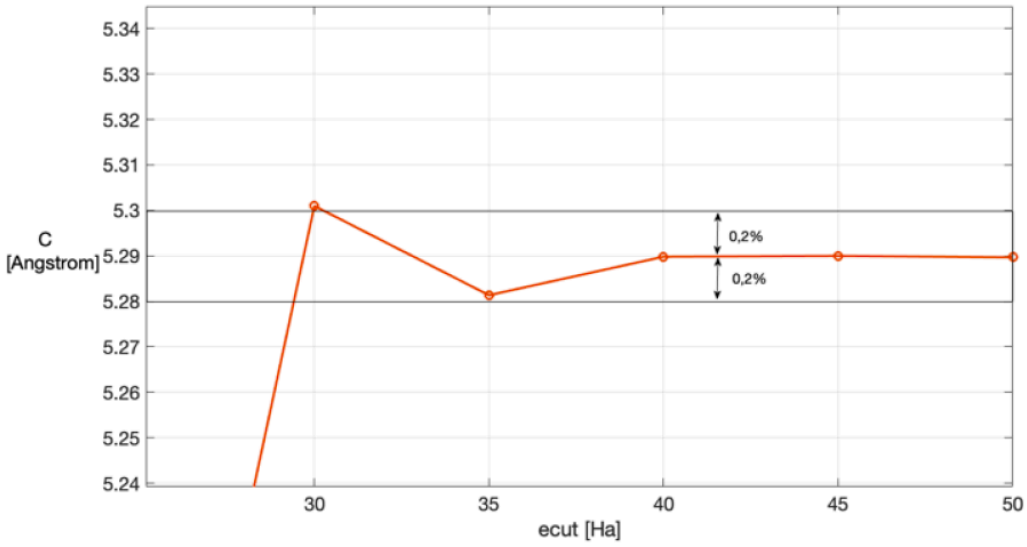


B. Total energy as a function of wavevector sampling

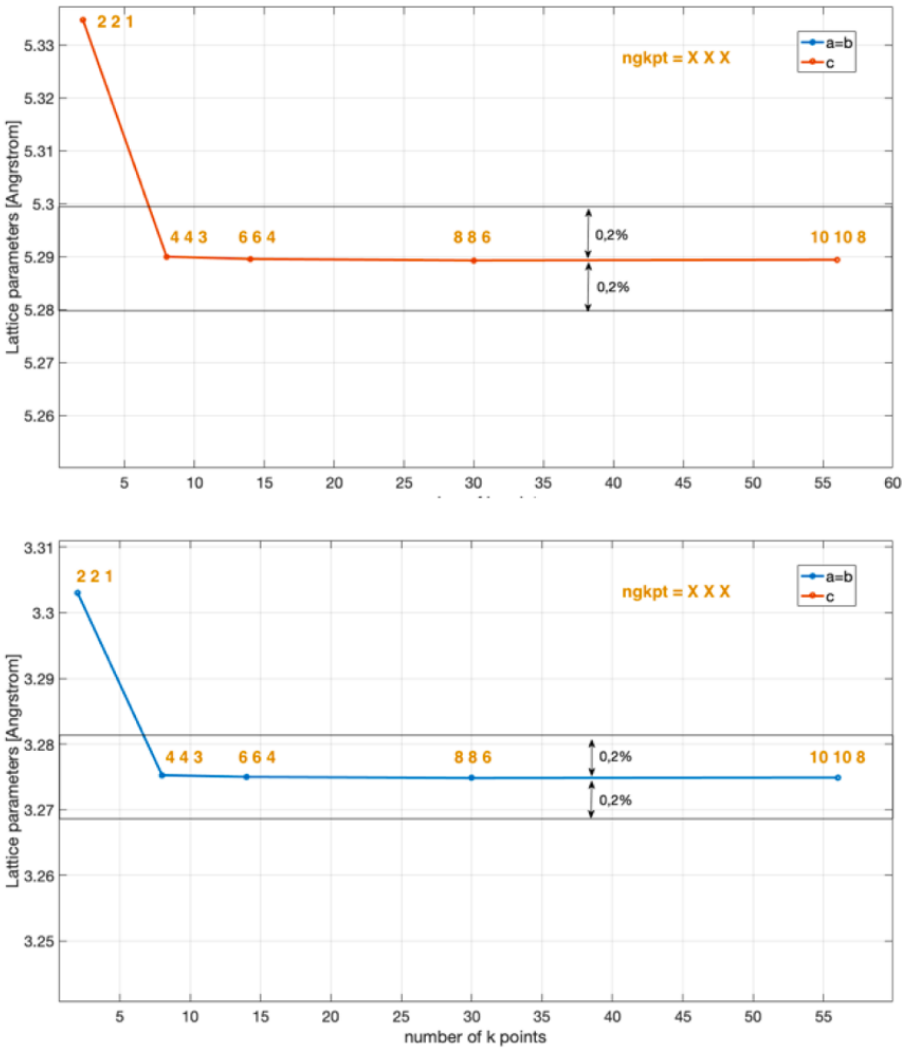


C. Cell parameters as a function of planewave cut-off energy





D. Cell parameters as a function of wavevector sampling



E. or F. Electronic band structure