Project A20
FYS-MENA4111

Erlend Tiberg North & Alexandra Jahr Kolstad

20. november 2020
Week 44-

Abstract

Innhold

Ting å gjøre:

- lage en mappe på saga for begge

  done

- skaffe POSCAR, jobfile og INCAR (de andre følger fra disse)

  done

- sjekke at den konvergerer (decent ENCUT og KPOINTS)

  done

  The data shows that we should use 450eV for ENCUT as that is the 1st job with a difference less than 3meV.

  For k-density we see that even the lowest value, 1.0, is within 3 meV (1.0 gives around 1.75 meV), so this can be used. However, the data shows that 3.0 is below 1 meV, with 4.0 being identical in energy to 5.0. This can possibly be discussed in group, but 1.0 should technically be enough for k-density.

- relaxe POSCAR og static etter relax POSCAR

  done

- total og relativ energi (fra static etter relax)

  done

- DOS (båndgap) og LDOS (båndstruktur)

  done

- romlig elektronstruktur; 3D-plot av ladningstetthet (VESTA)
- bytte ut hydrogen i alkoholgruppen med lantanoidatomer (Yb, Nd, Tm og Y)
- relaxe POSCAR og static etter relax POSCAR
- total og relativ energi (fra static etter relax)
- DOS (båndgap) og LDOS (båndstruktur)
- romlig elektronstruktur; 3D-plot av ladningstetthet (VESTA)

Ting å ha i LaTeX:

- abstrakt
- kort introduksjon av materialet
- kort om metode, valg av paramtere (CUTOFF, etc)
- presentasjon av de viktigste resultatene
- diskusjon av hvordan resultatene kan tolkes, f.eks. sammenligne til eksperimenter eller tidligere beregninger i litteraturen
- konklusjon/oppsummering
- kilder
- appendix ?

OBS: husk å lagre bilder for rapporten og presentasjonen mens man gjør beregningene

1 Introduction

2 Method

2.1 Energy convergence

ENCUT: 300 to 900

2.2 K-points convergence

K-point density: 1.0 to 6.0

3 Results

3.1 Energy convergence

Started to convergence around 450 eV for ENCUT.

3.2 K-points convergence

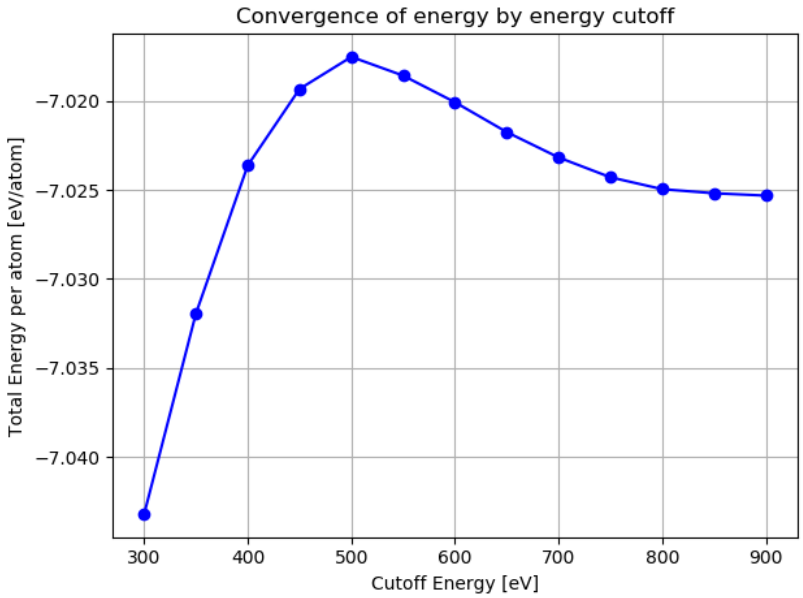
4 Discussion

5 Conclusion

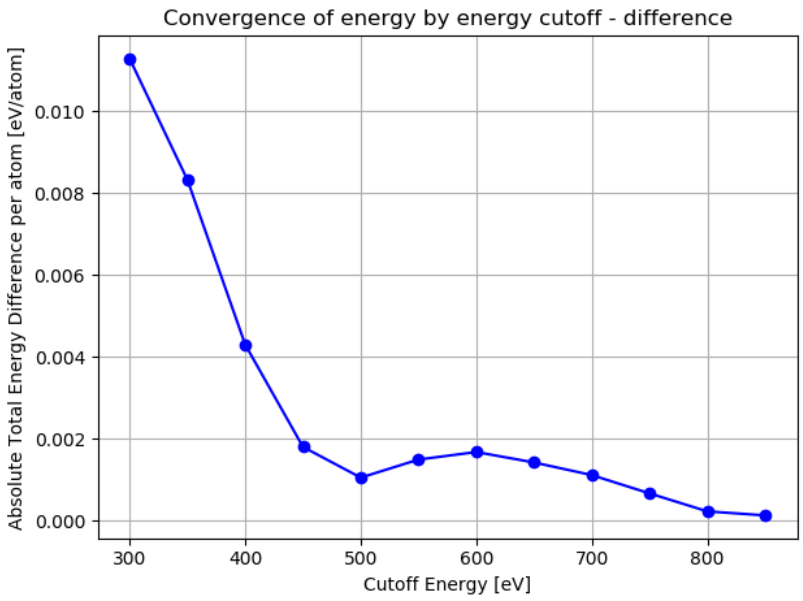
6 References

[1] Ben G. Streetman & Sanjay Kumar Banerjee, 2016, *Solid State Elctronic Devices seventh edition*, Pearson Education

A Convergence energy

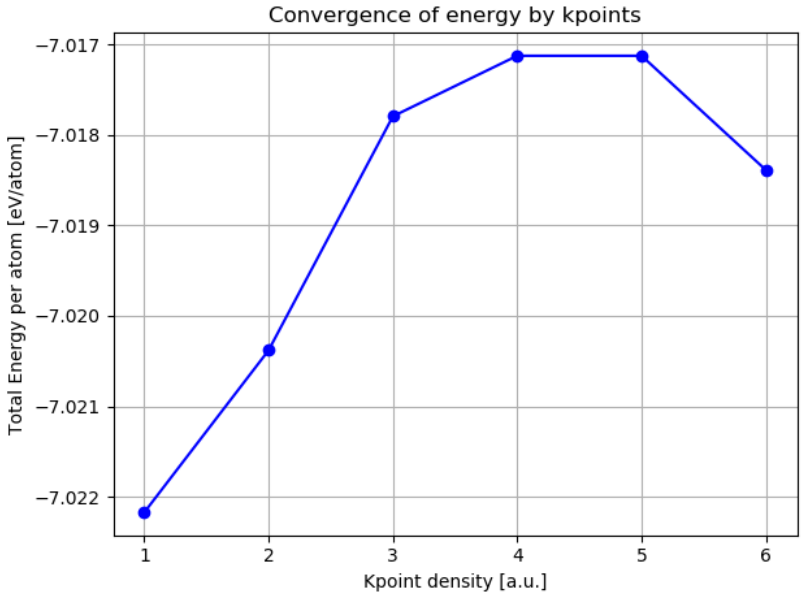


Figur 1: .

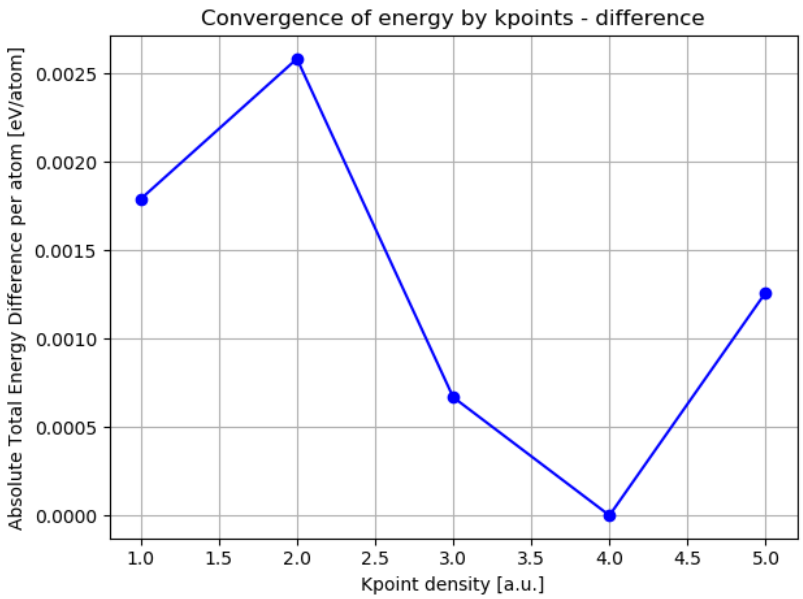


Figur 2: .

B Convergence kpoints

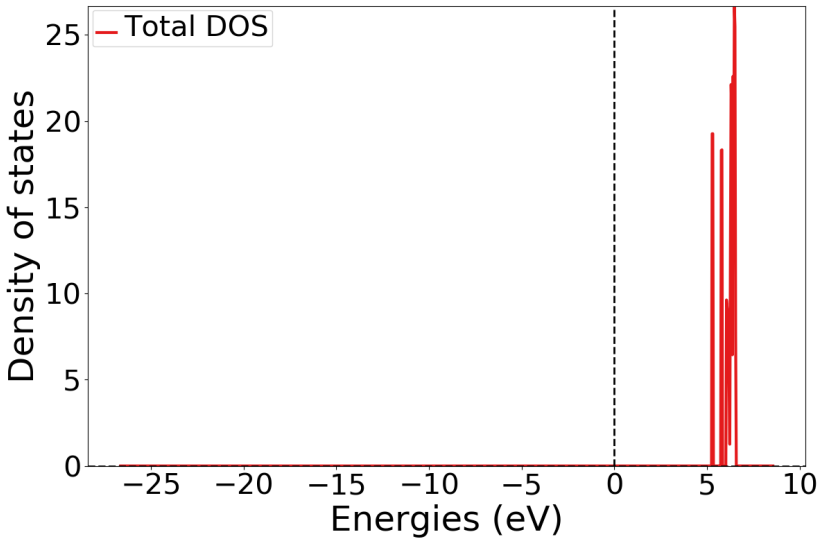


Figur 3: .

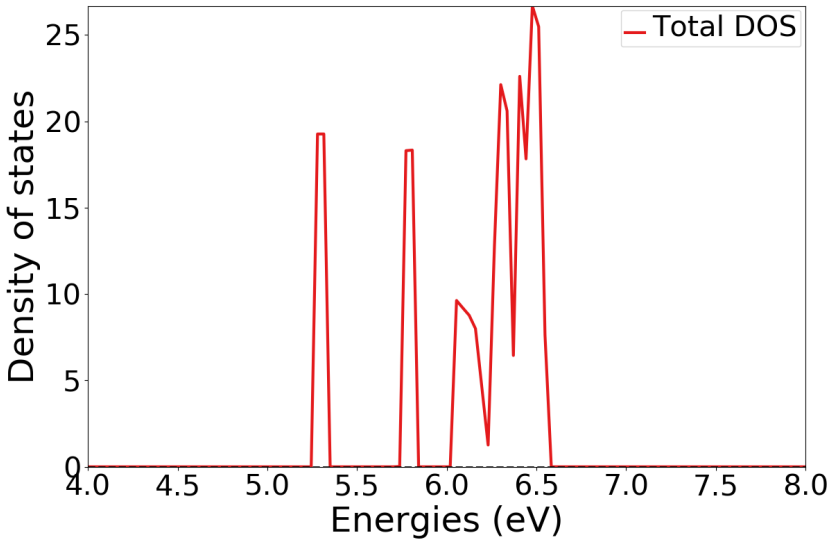


Figur 4: .

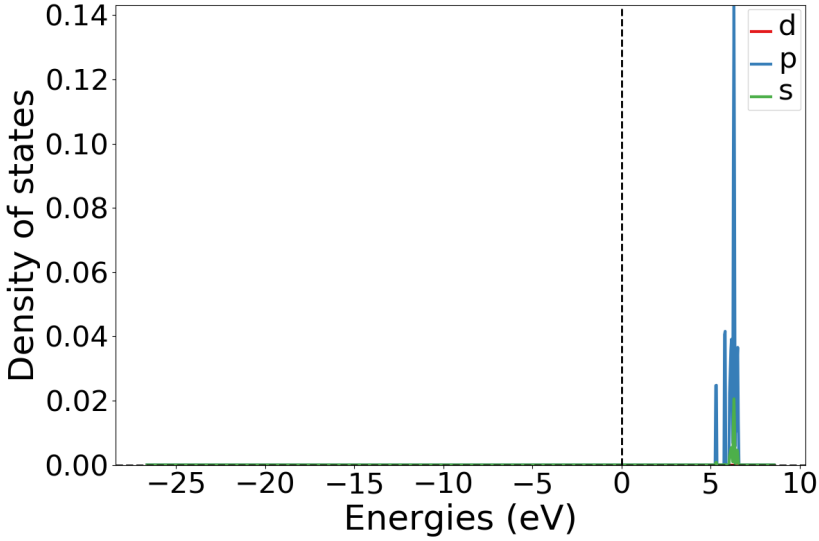
C DOS-bilder



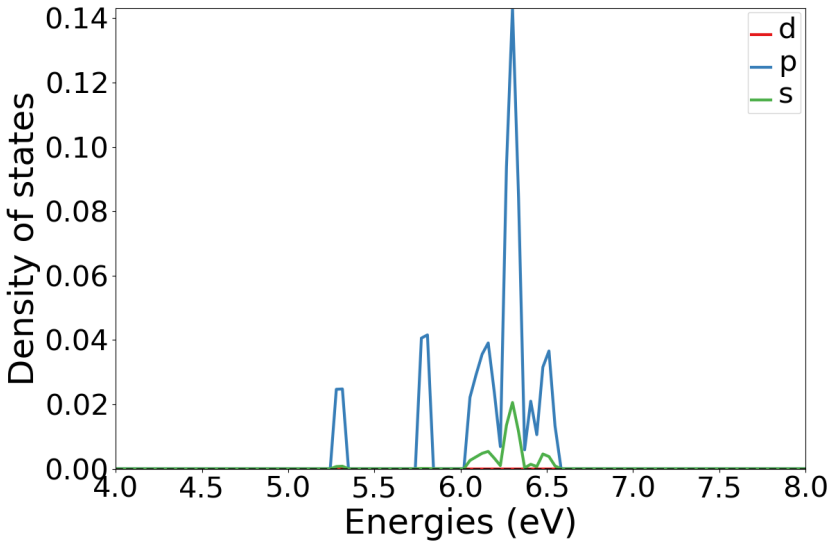
Figur 5: .



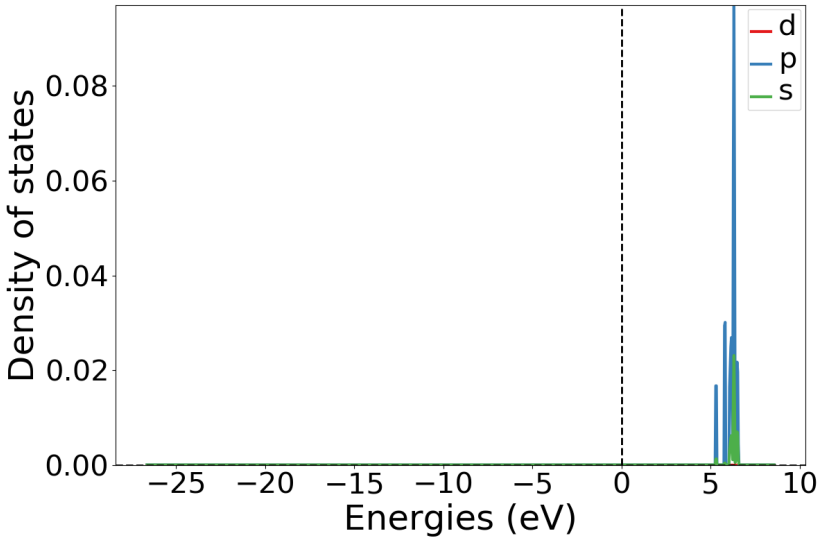
Figur 6: .



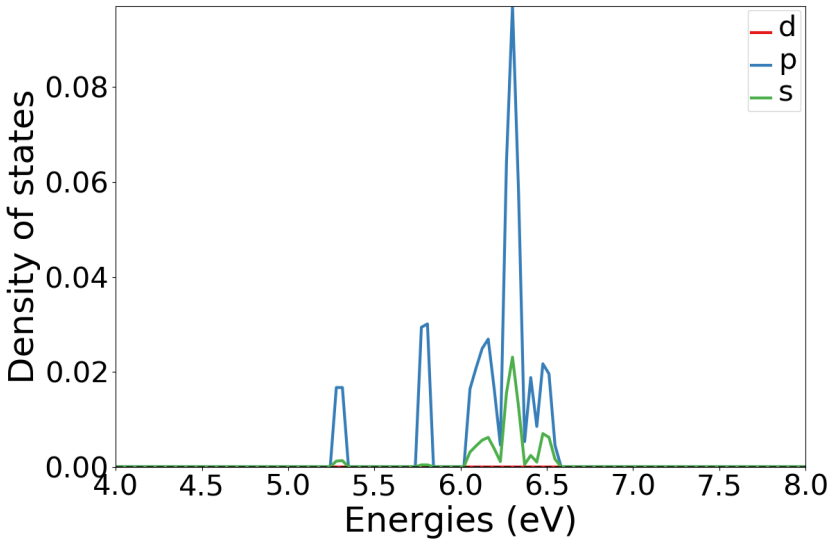
Figur 7: .



Figur 8: .

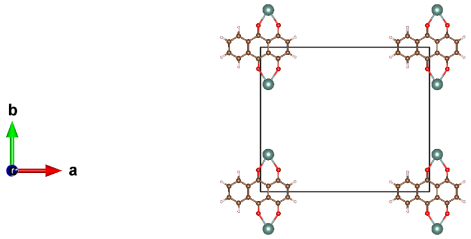


Figur 9: .

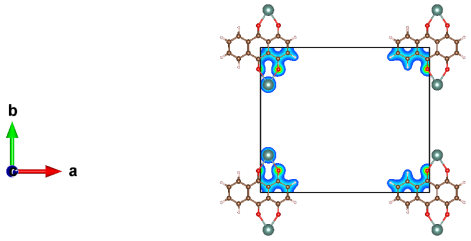


Figur 10: .

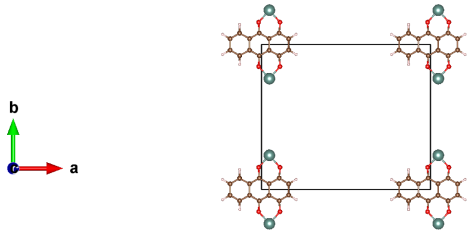
D Y-bilder



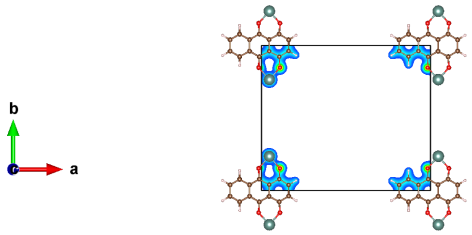
Figur 11: .



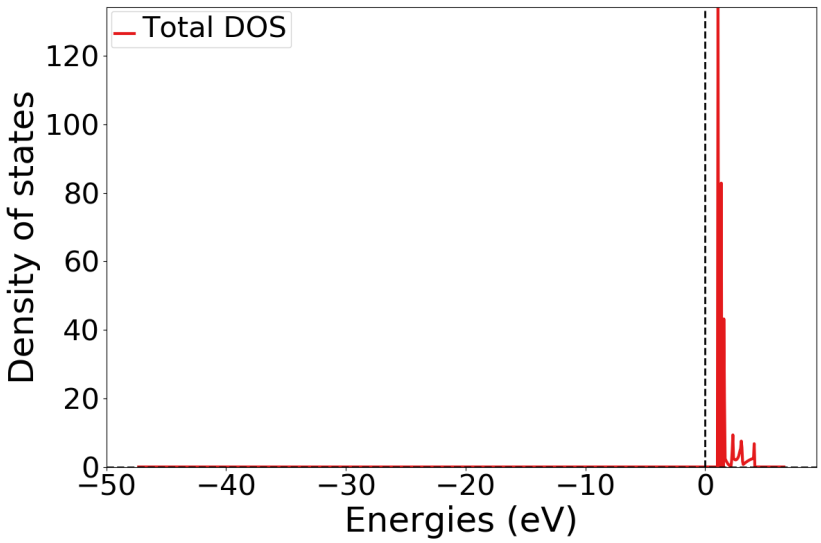
Figur 12: .



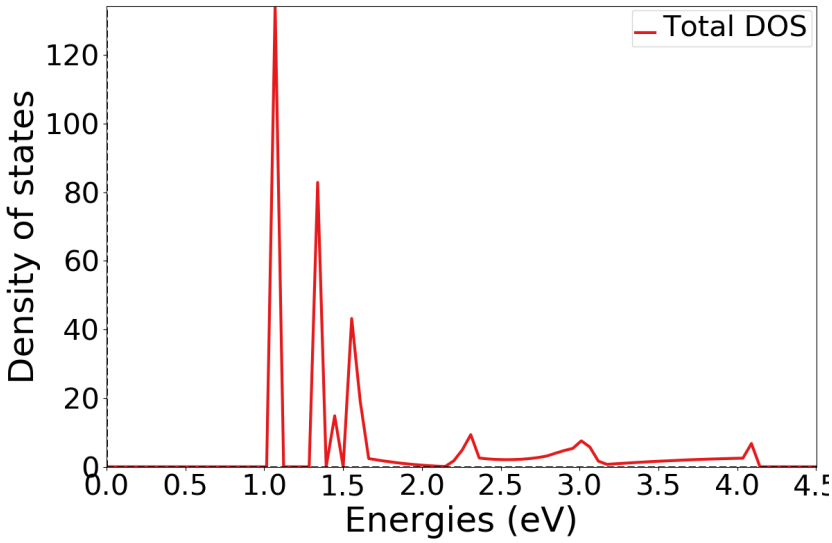
Figur 13: .



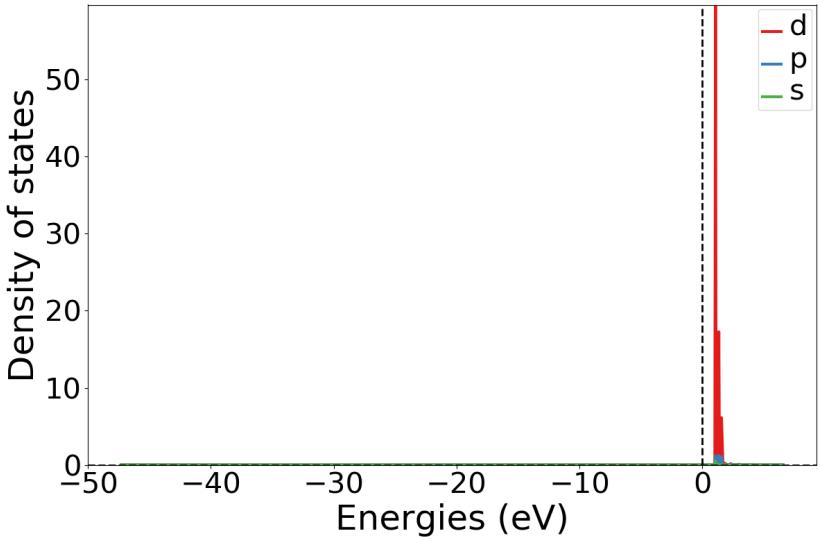
Figur 14: .



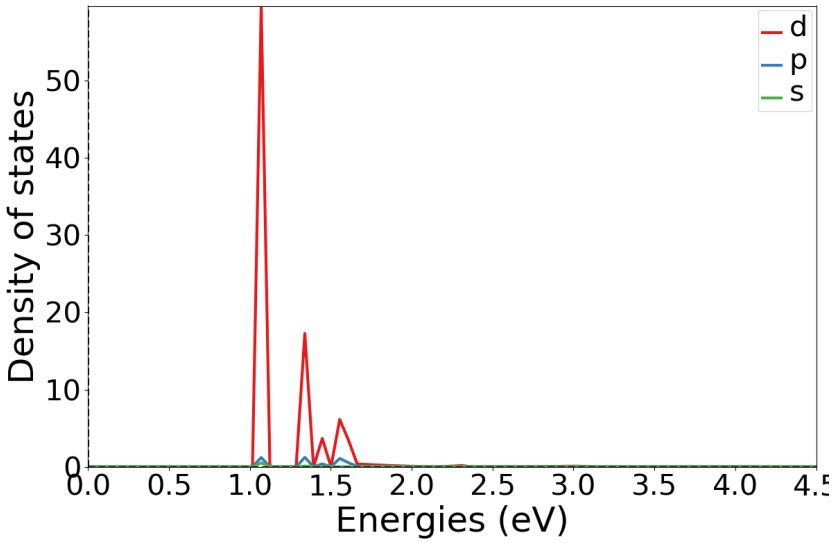
Figur 15: .



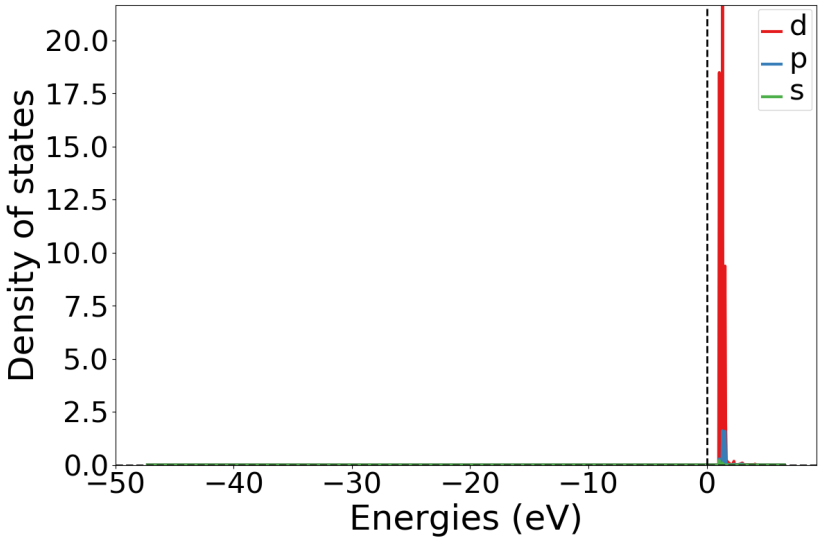
Figur 16: .



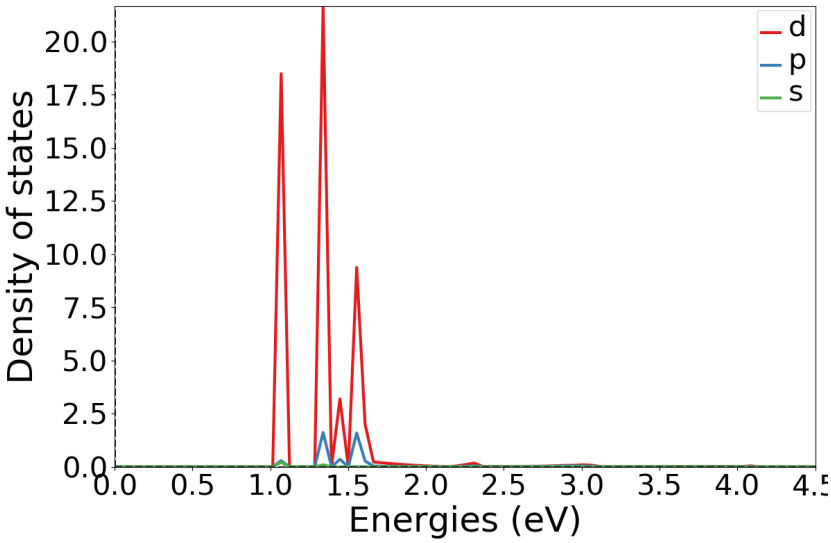
Figur 17: .



Figur 18: .

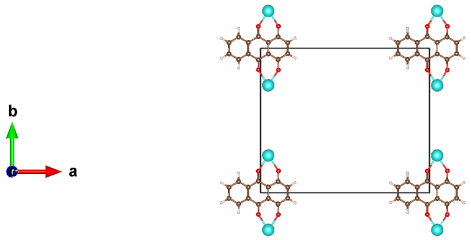


Figur 19: .

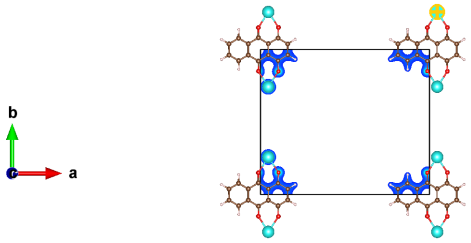


Figur 20: .

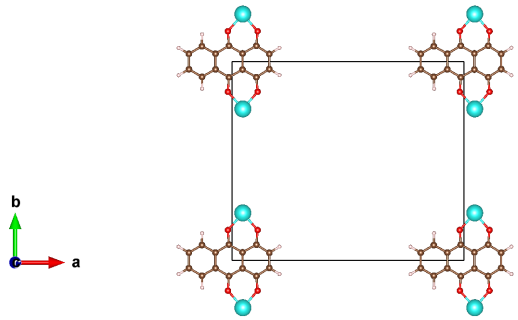
E Yb-bilder



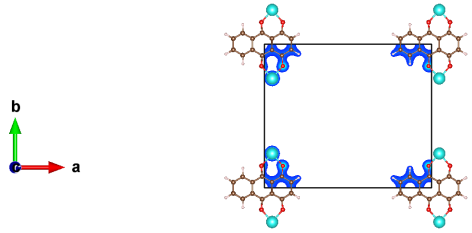
Figur 21: .



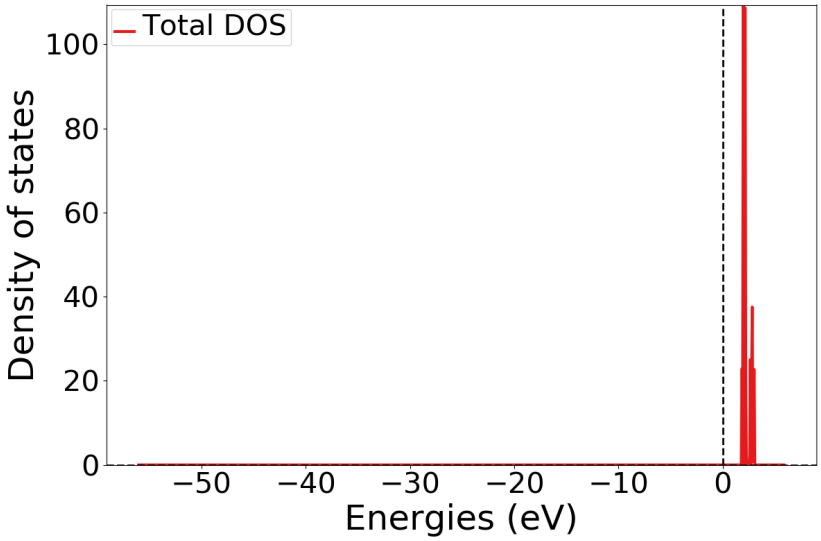
Figur 22: .



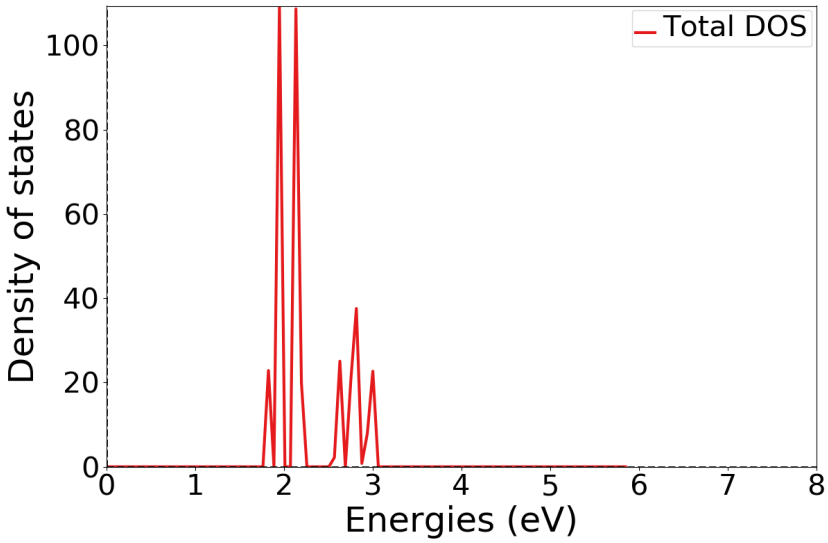
Figur 23: .



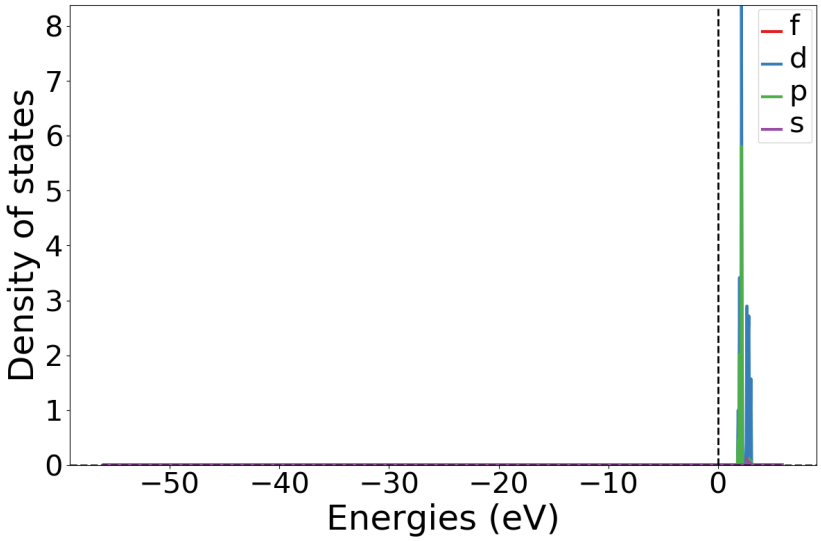
Figur 24: .



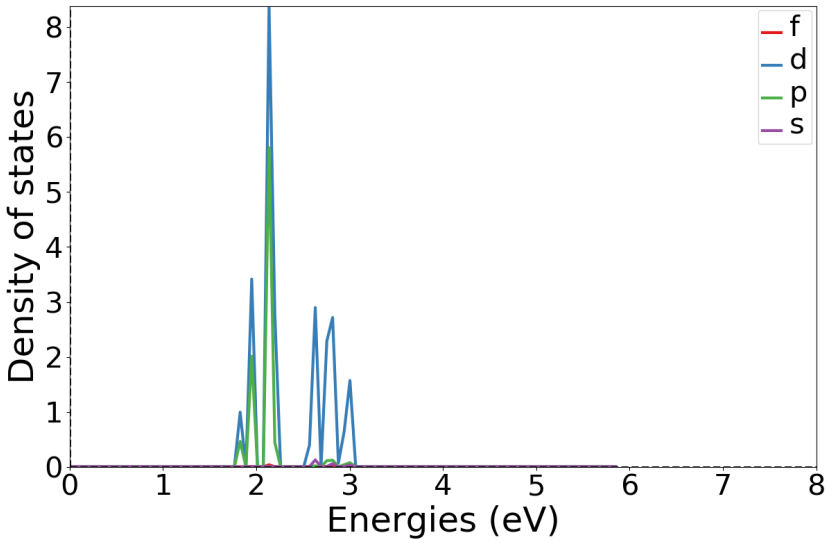
Figur 25: .



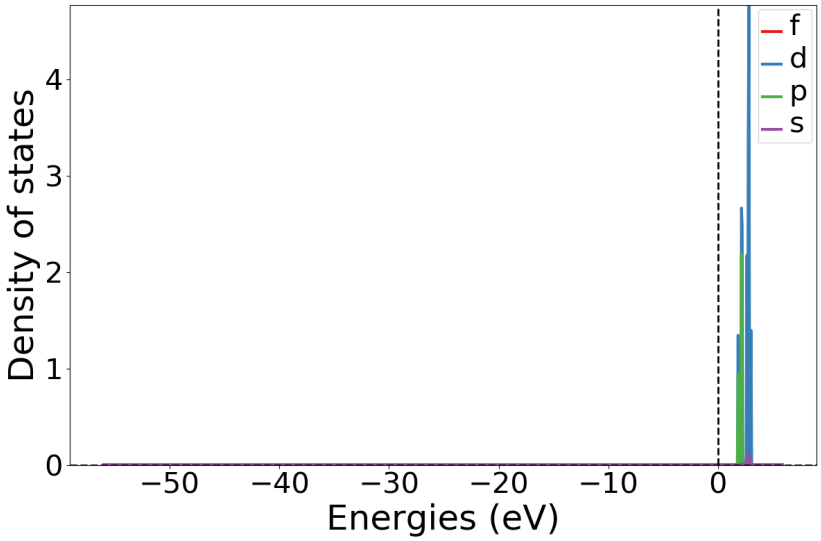
Figur 26: .



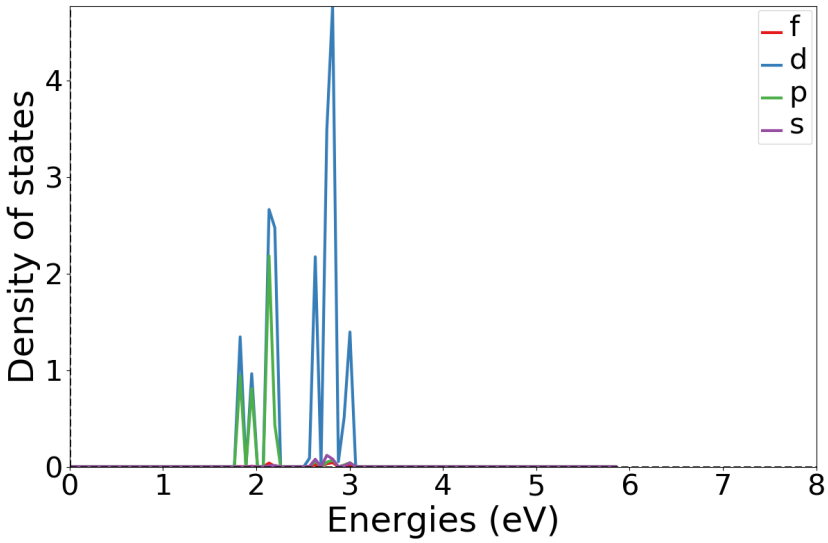
Figur 27: .



Figur 28: .



Figur 29: .



Figur 30: .

F Appendix 2