

Project A20
FYS-MENA4111

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Week 44-

Abstract

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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.

- relax 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 L^AT_EX:

- 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

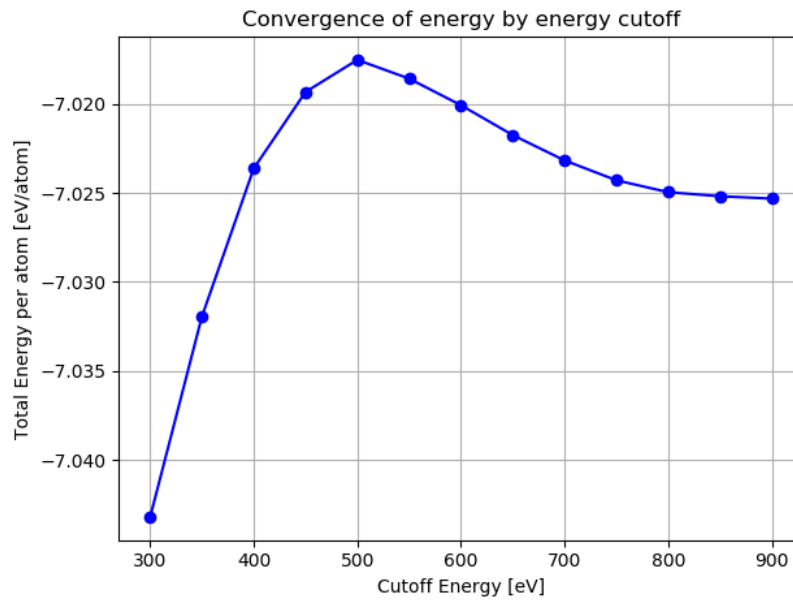


Figure 1: .

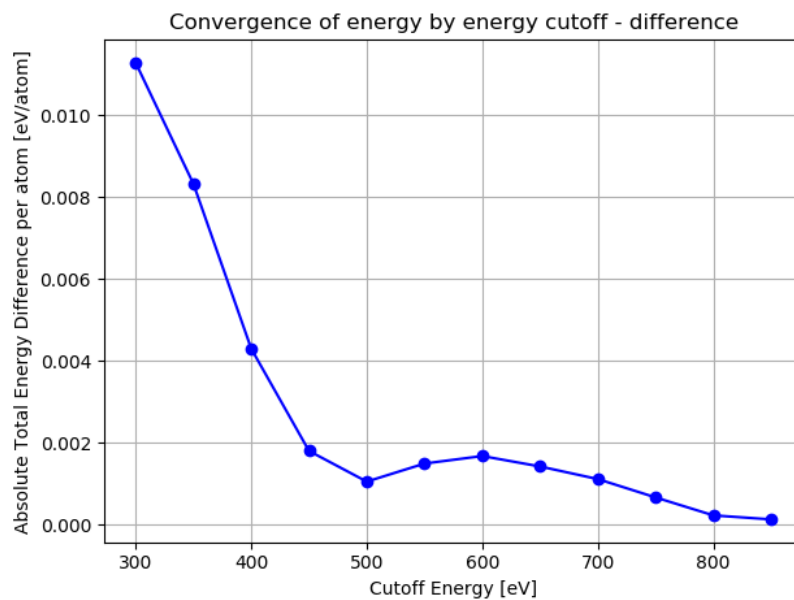


Figure 2: .

B Convergence kpoints

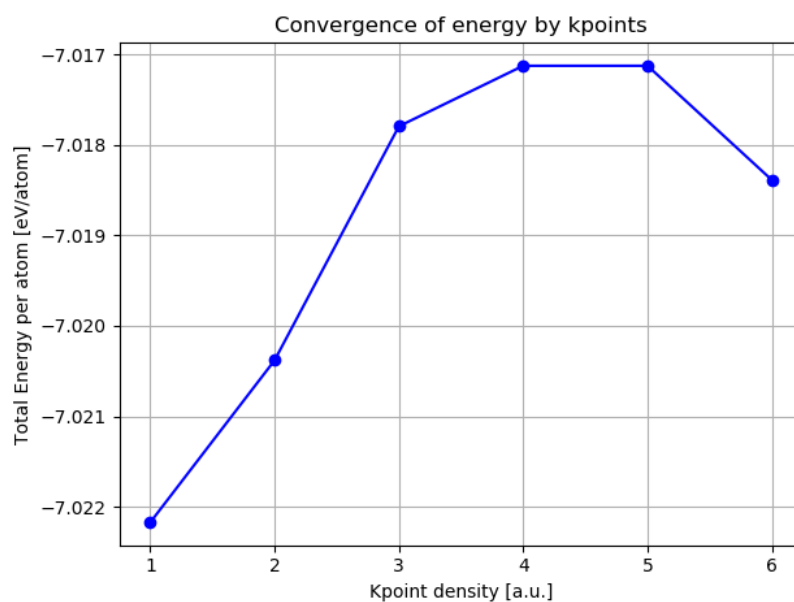
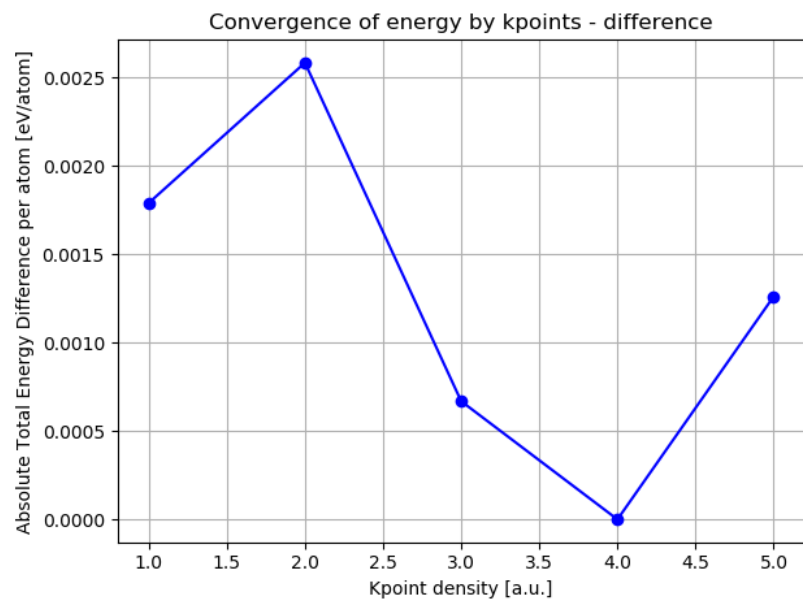
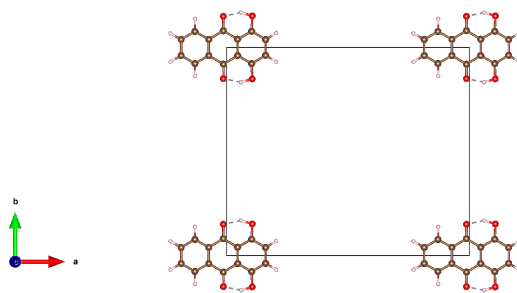


Figure 3: .



Figur 4: .

C Quinizarin-bilder



Figur 5: .

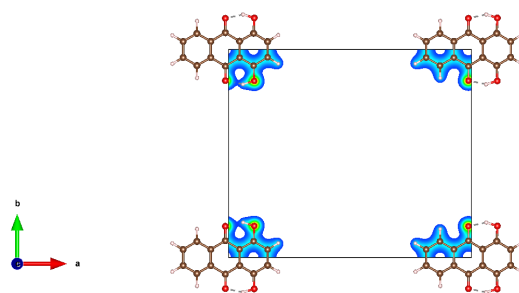


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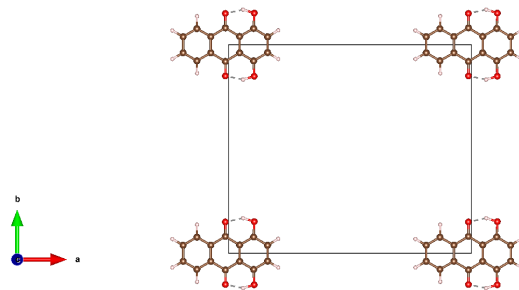


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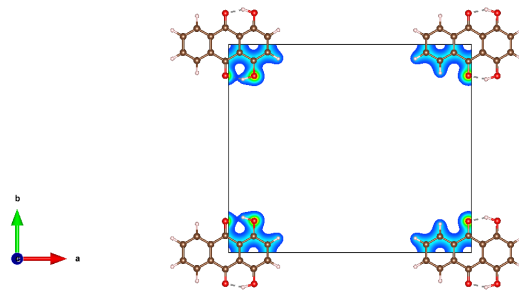
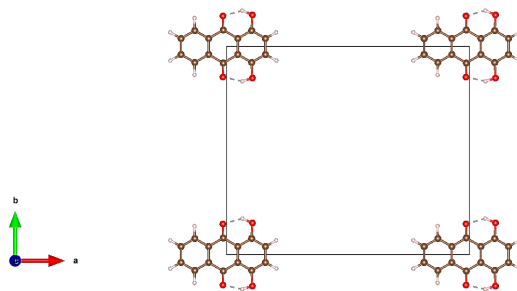
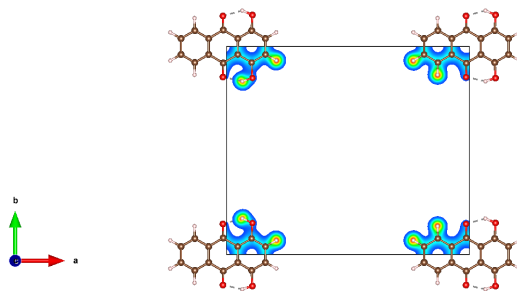


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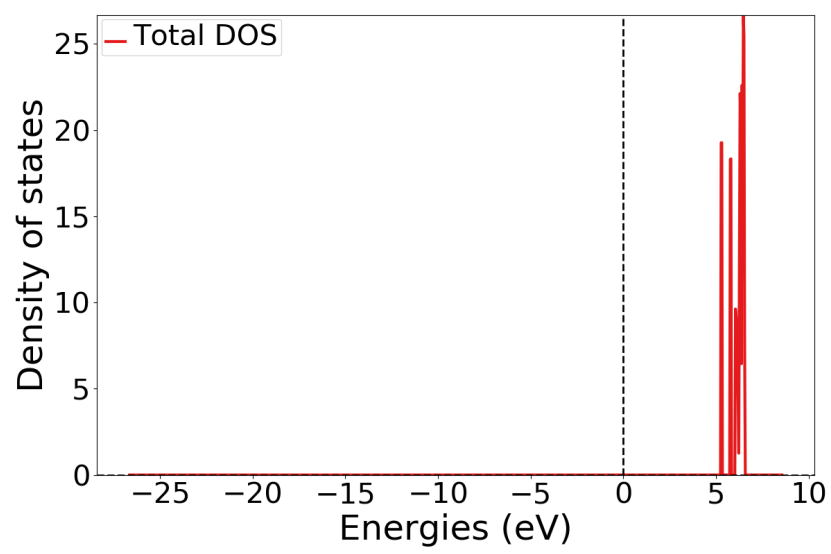
D DOS-bilder



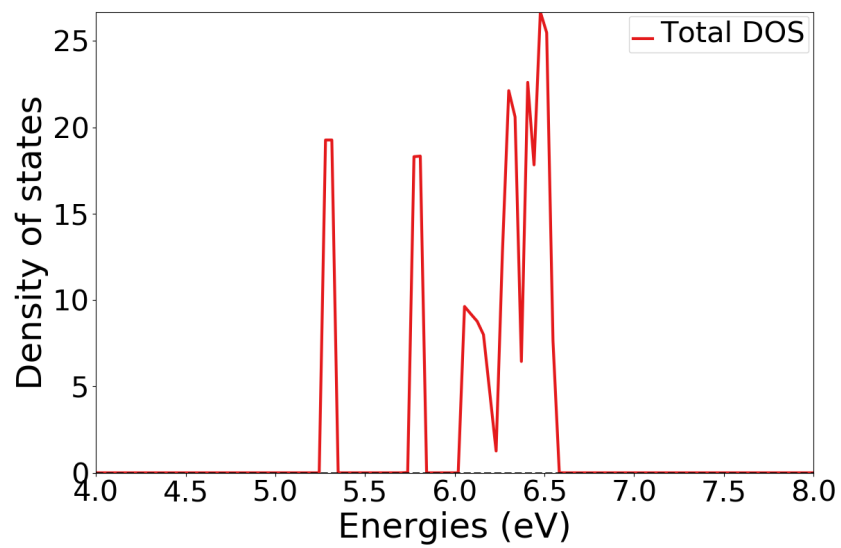
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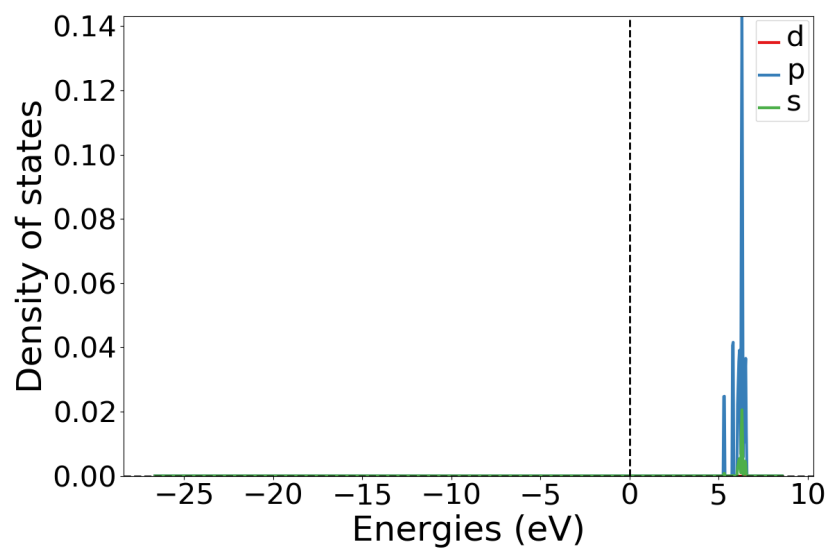
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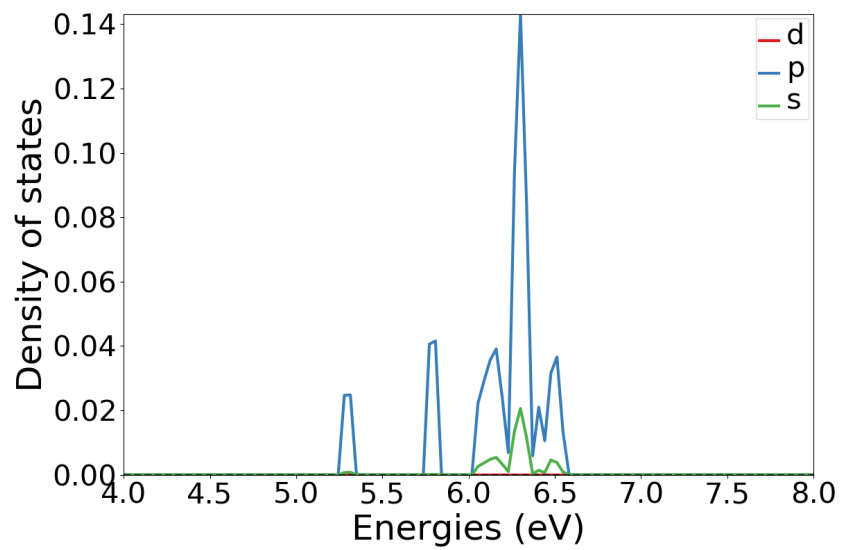
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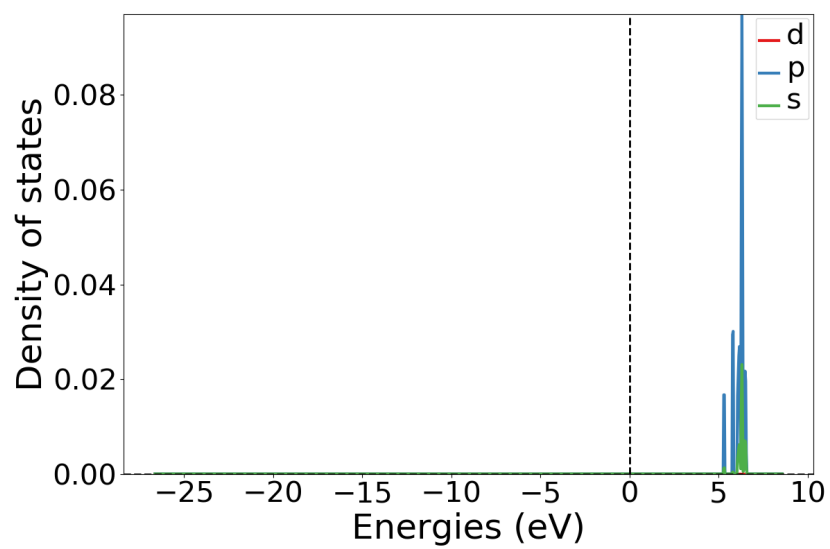
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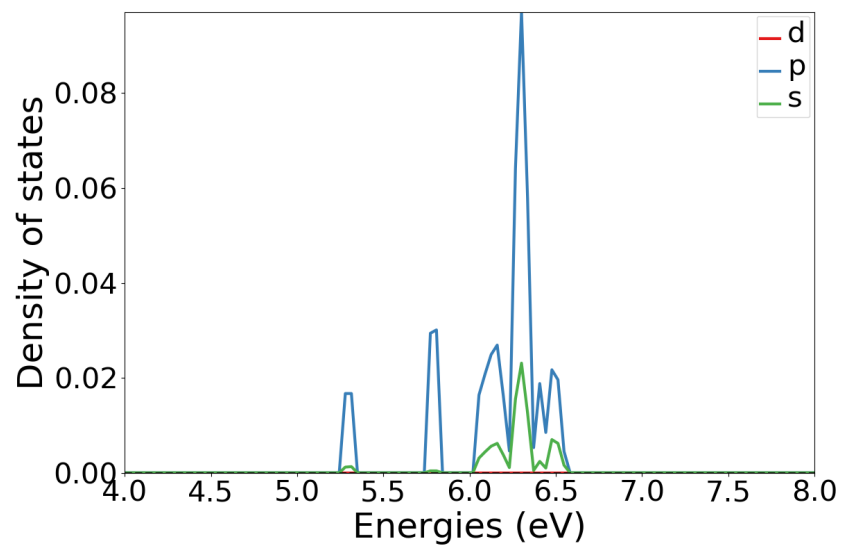
Figur 13: .



Figur 14: .

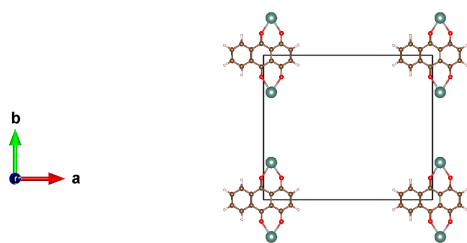


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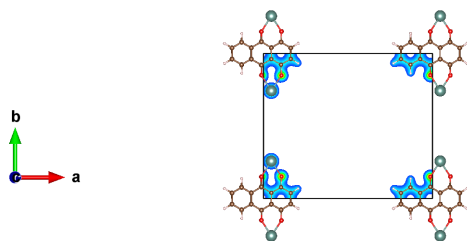


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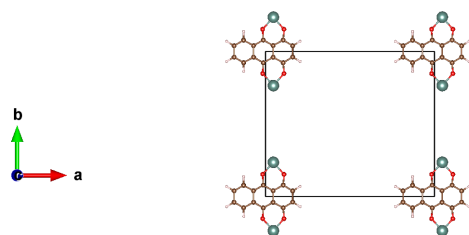
E Y-bilder



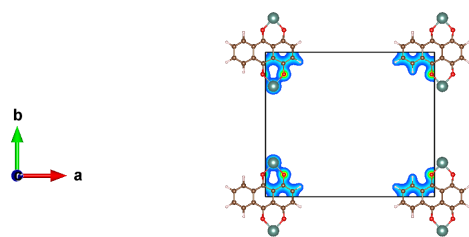
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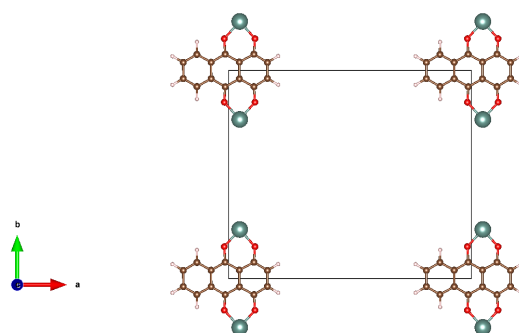
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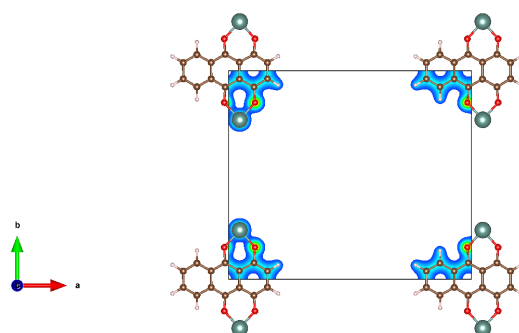
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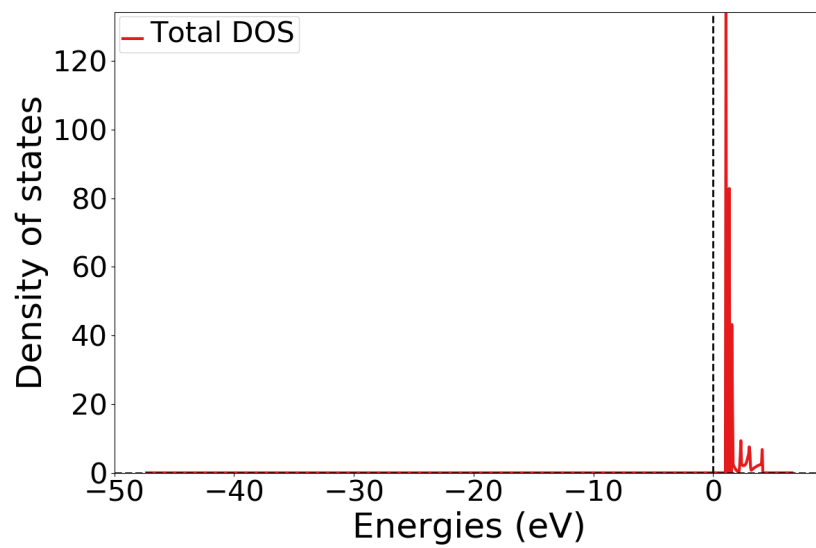
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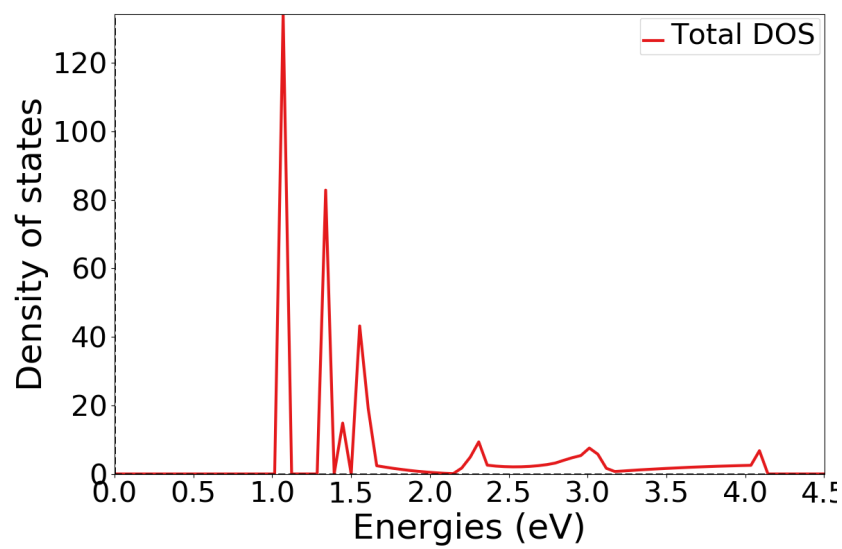
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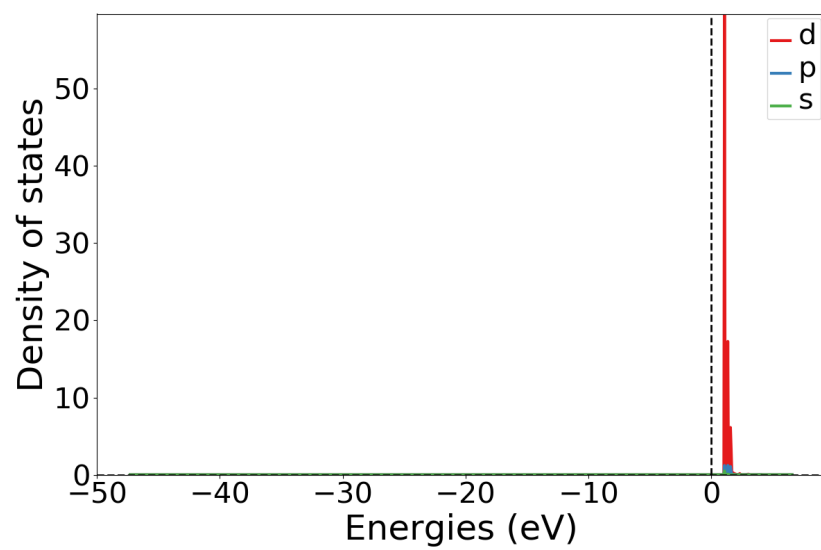
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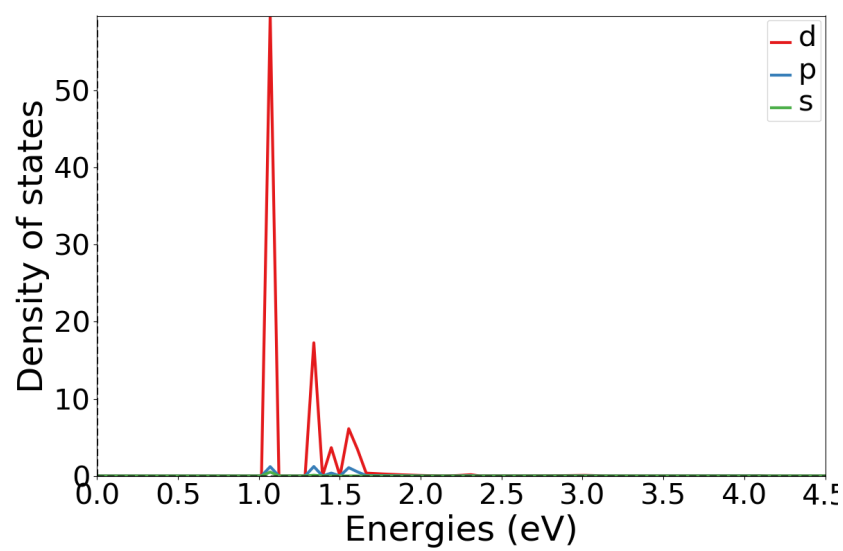
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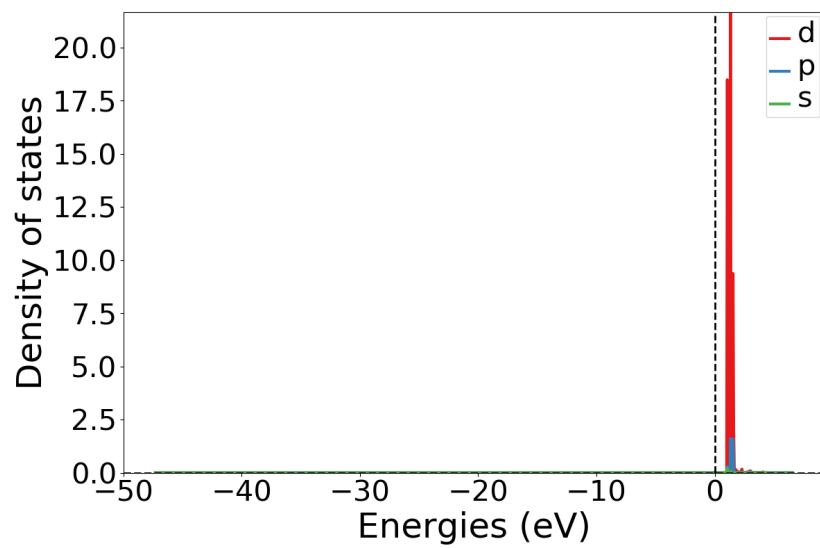
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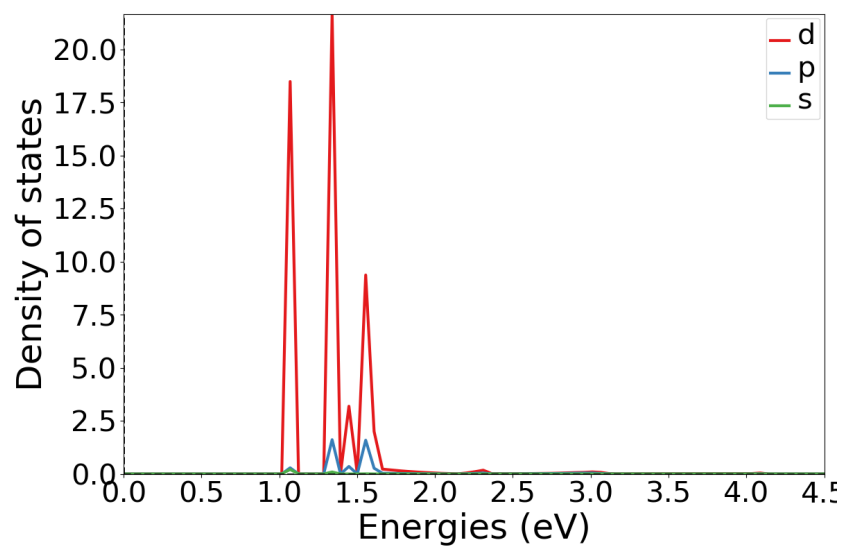
Figur 25: .



Figur 26: .

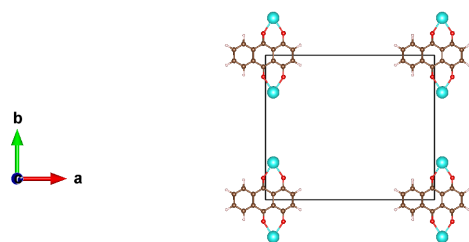


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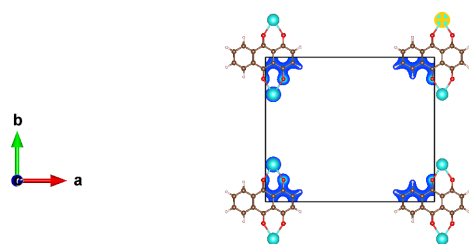


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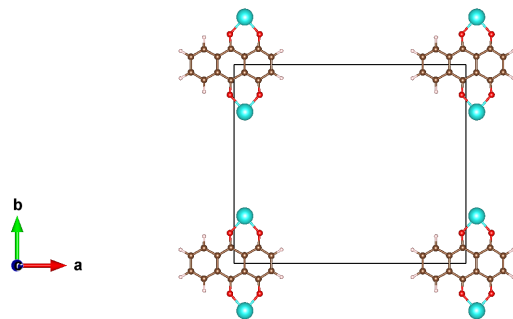
F Yb-bilder



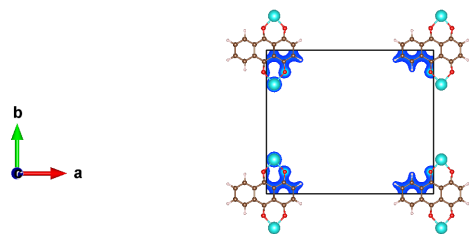
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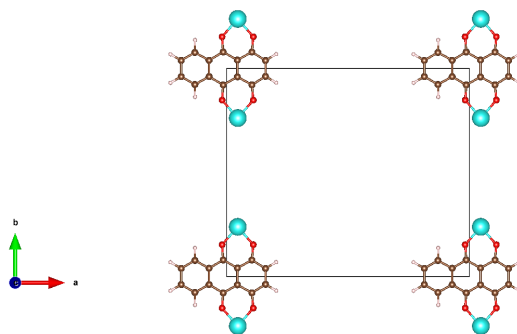
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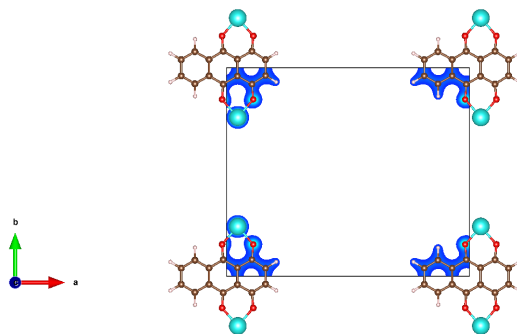
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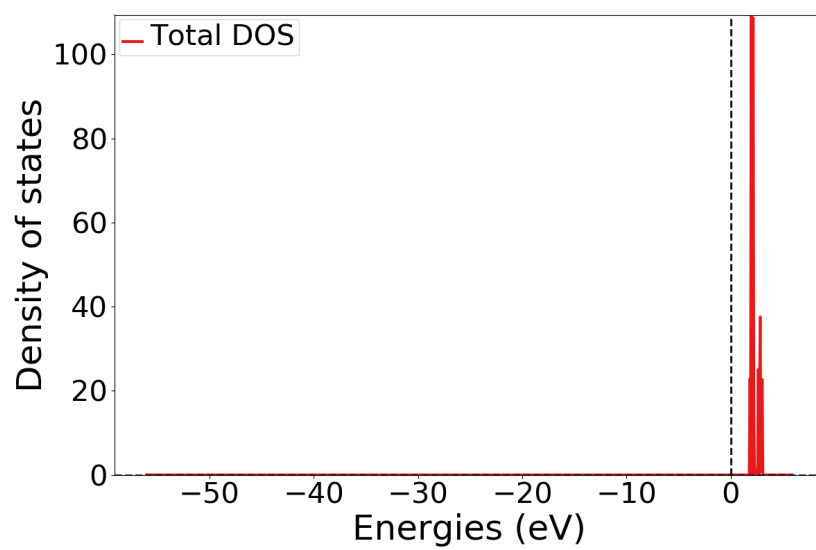
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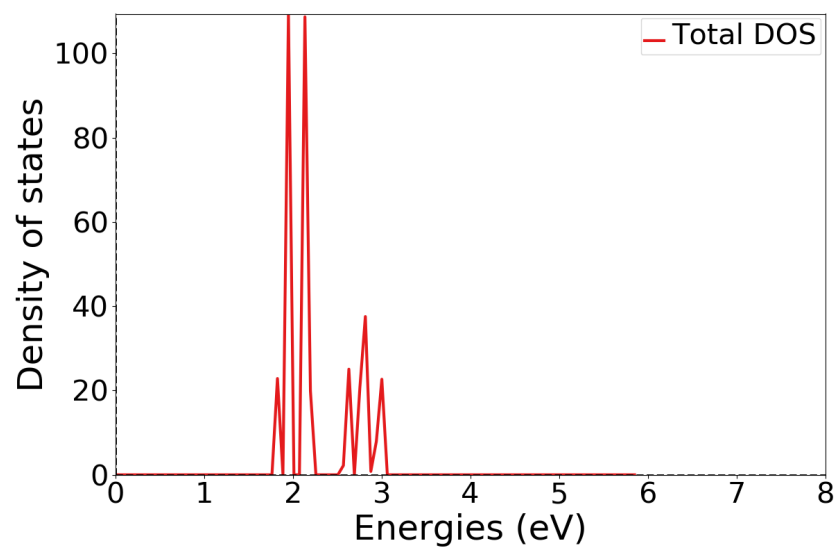
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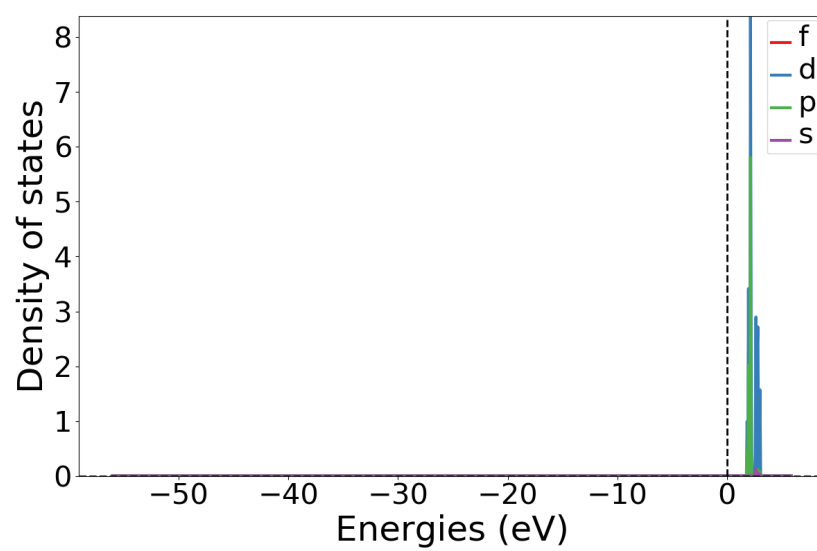
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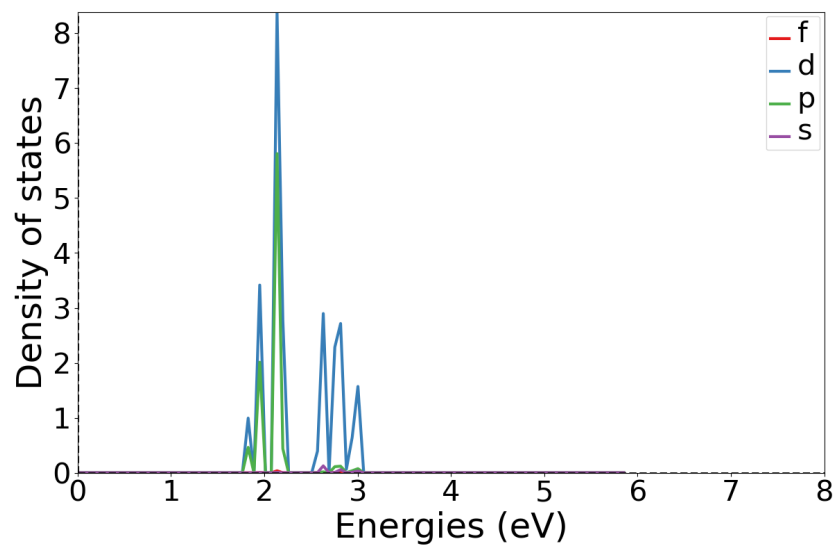
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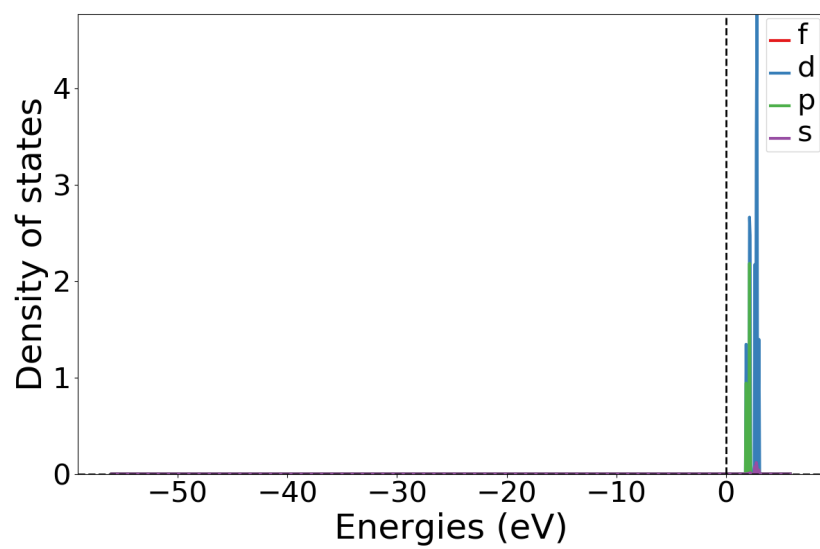
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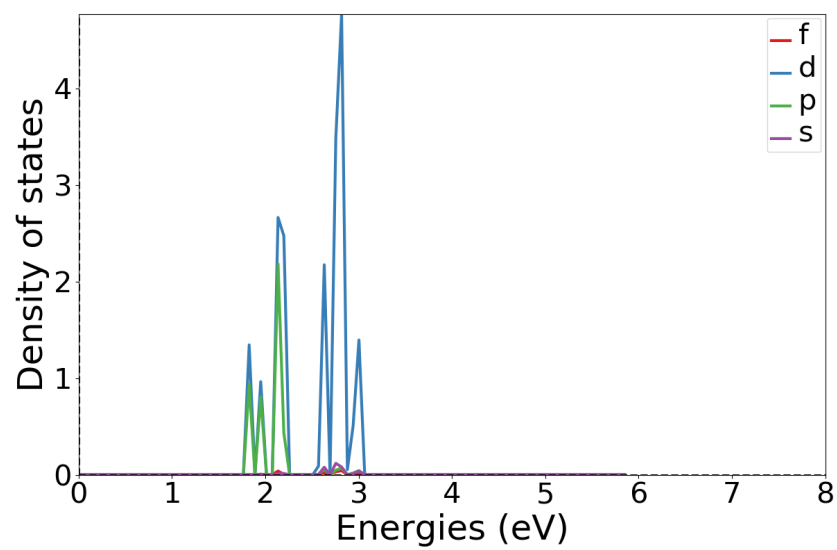
Figur 37: .



Figur 38: .



Figur 39: .



Figur 40: .

G Appendix 2