Project A20
FYS-MENA4111

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21. 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

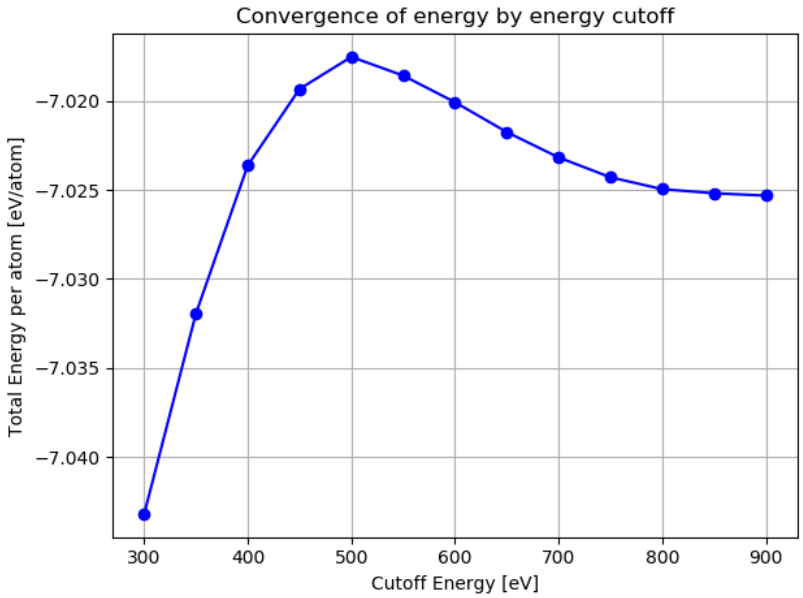
4 Discussion

5 Conclusion

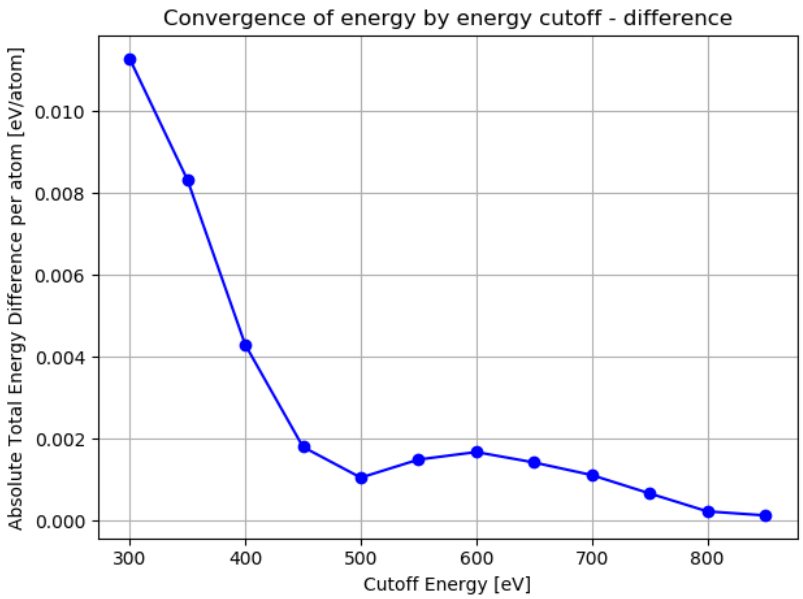
6 References

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

A Convergence energy

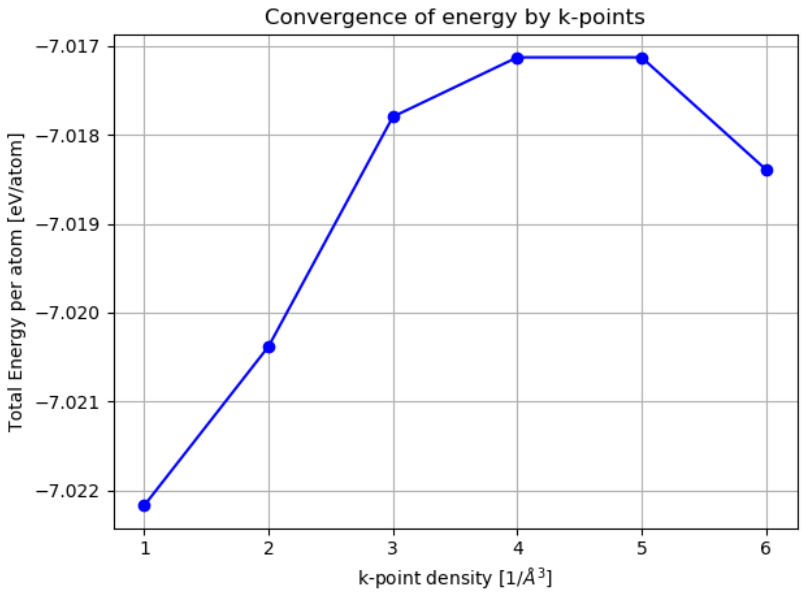


Figur 1: Plot of energy convergence for Quinizarin, with ENCUT ranging from 300 eV to 900 eV.

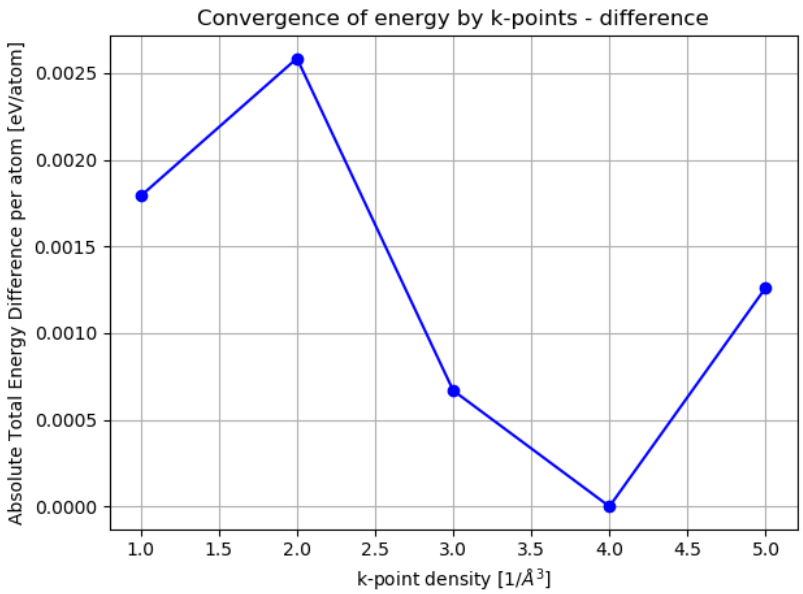


Figur 2: Plot of the difference in energy convergence for Quinizarin, given by ENCUT.

B Convergence k-points

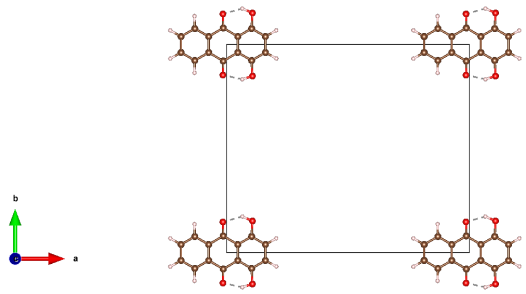


Figur 3: Plot of energy convergence for Quinizarin, with k-point density ranging from 1 to 6.

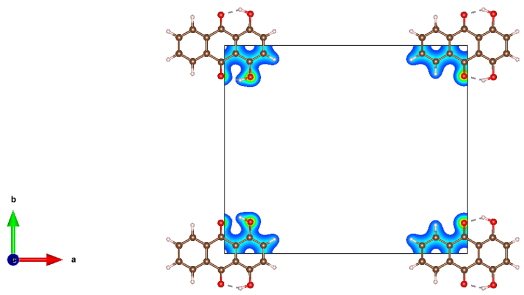


Figur 4: Plot of the difference in energy convergence for Quinizarin, given by k-point density.

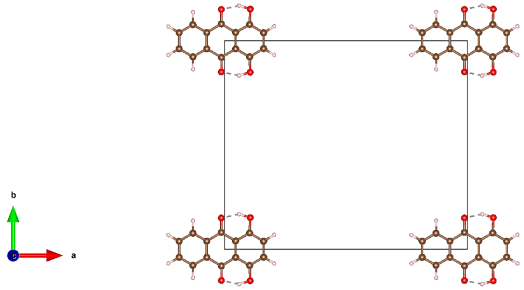
C Quinizarin-bilder



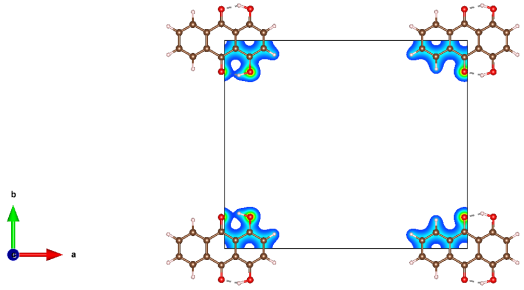
Figur 5: Structure of Quinizarin for static VASP calculation.



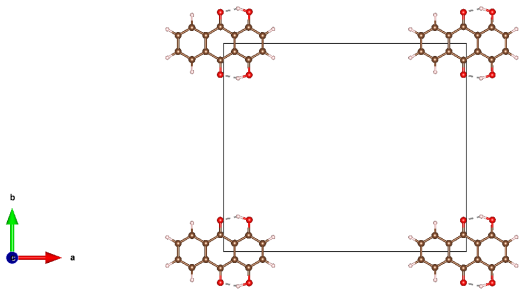
Figur 6: Charge density of Quinizarin for static VASP calculation.



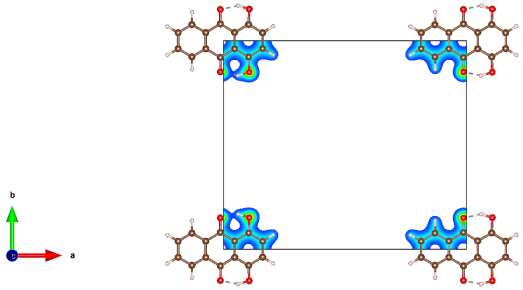
Figur 7: Structure of Quinizarin for relaxed VASP calculation.



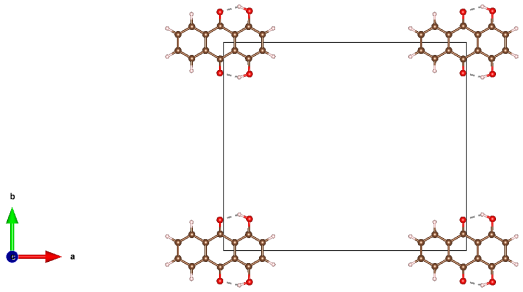
Figur 8: Charge density of Quinizarin for relaxed VASP calculation.



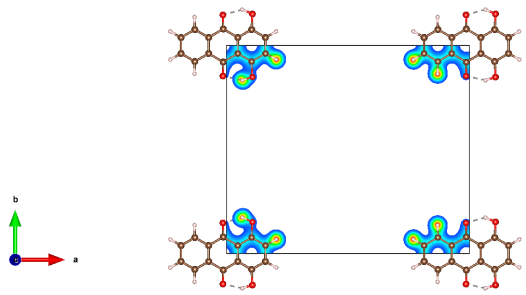
Figur 9: Structure of Quinizarin for static VASP calculation after relaxed calculation.



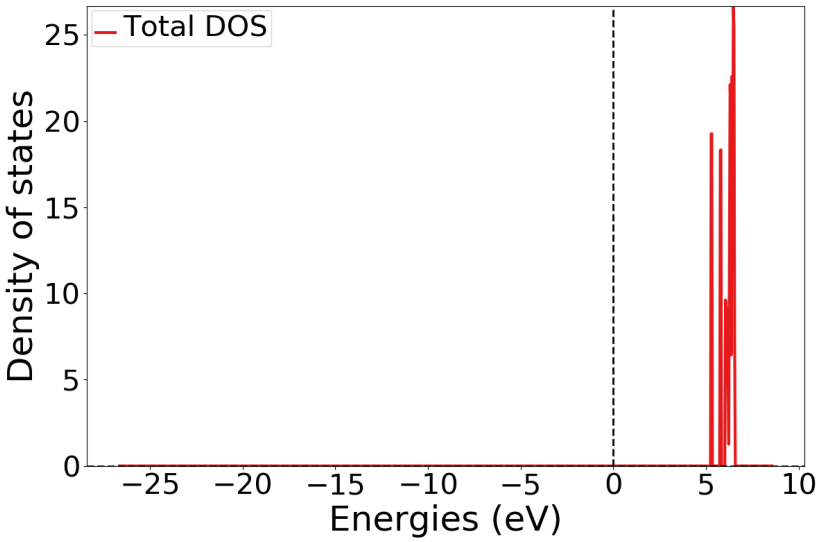
Figur 10: Charge density of Quinizarin for static VASP calculation after relaxed calculation.



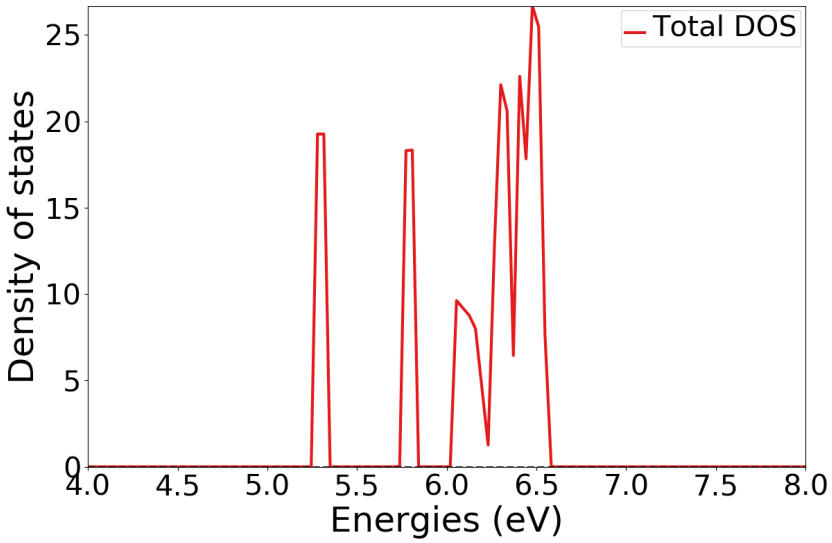
Figur 11: Structure of Quinizarin for DOS VASP calculation.



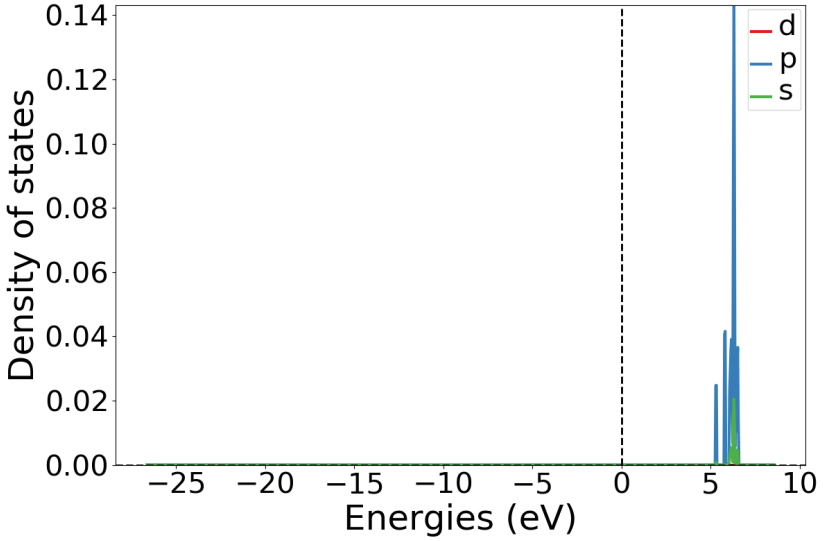
Figur 12: Charge density of Quinizarin for DOS VASP calculation.



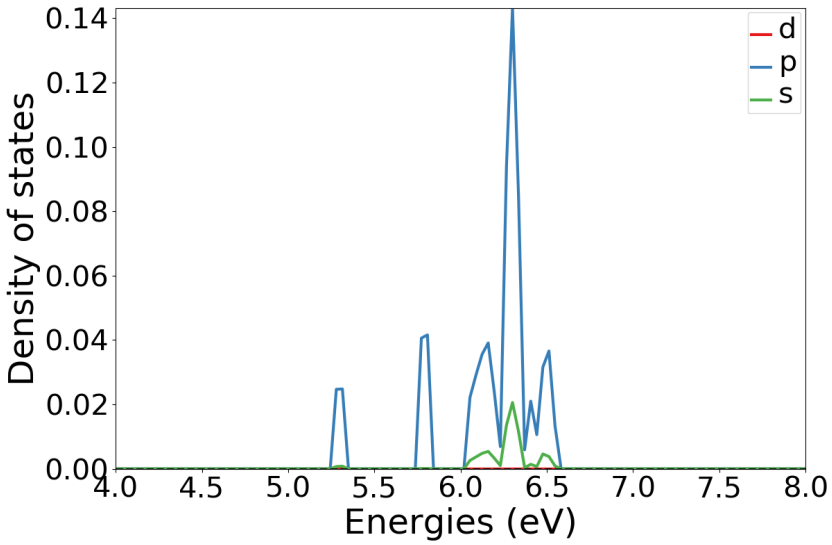
Figur 13: Plot of total DOS for Quinizarin.



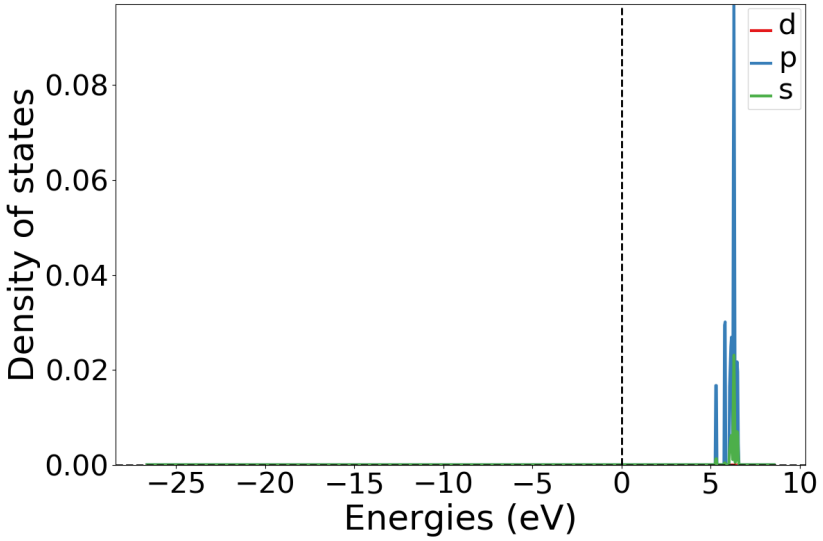
Figur 14: Plot of total DOS for Quinizarin, zoomed in for energies between 4.0 eV and 8.0 eV.



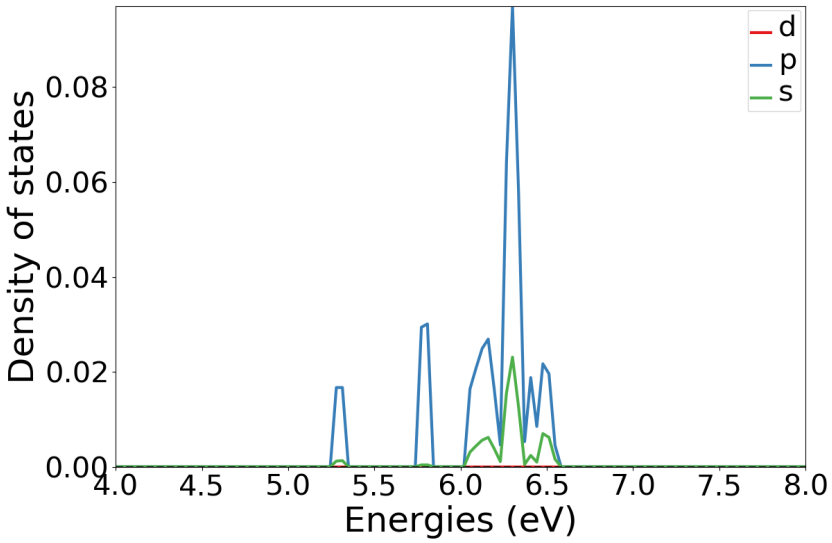
Figur 15: Plot of local DOS for atom number 25(H in alcohol-group) for Quinizarin.



Figur 16: Plot of local DOS for atom number 25(H in alcohol-group) for Quinizarin, zoomed in for energies between 4.0 eV and 8.0 eV.

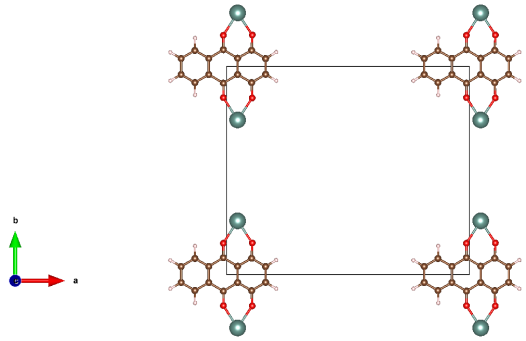


Figur 17: Plot of local DOS for atom number 26(H in alcohol-group) for Quinizarin.

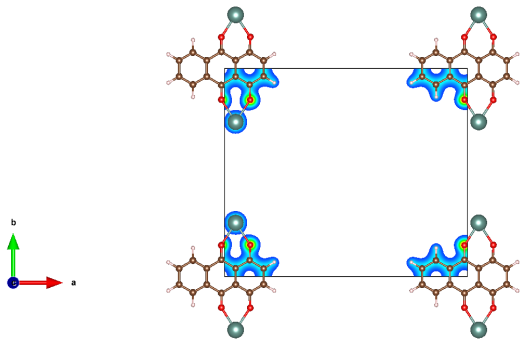


Figur 18: Plot of local DOS for atom number 26(H in alcohol-group) for Quinizarin, zoomed in for energies between 4.0 eV and 8.0 eV.

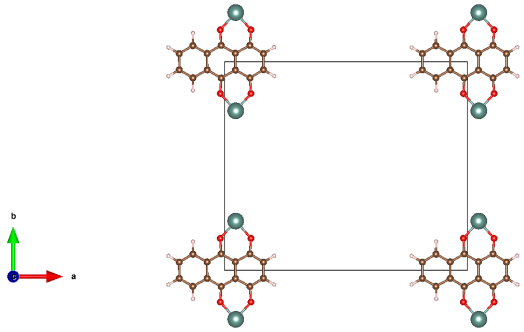
D Y-bilder



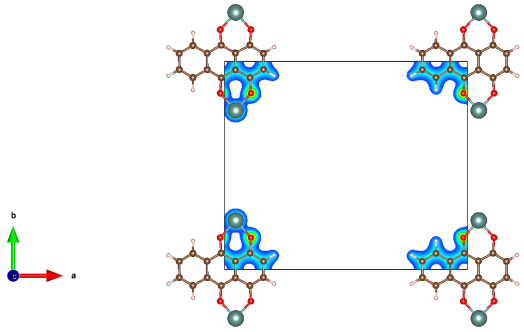
Figur 19: Structure of Quinizarin with Yttrium for static VASP calculation.



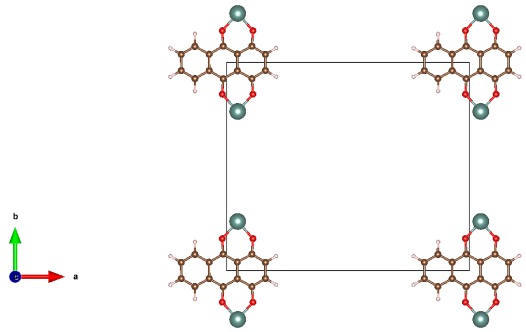
Figur 20: Charge density of Quinizarin with Yttrium for static VASP calculation.



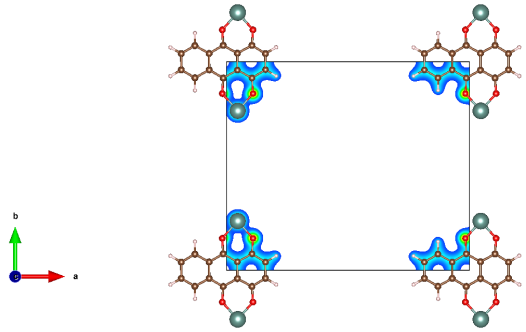
Figur 21: Structure of Quinizarin with Yttrium for relaxed VASP calculation.



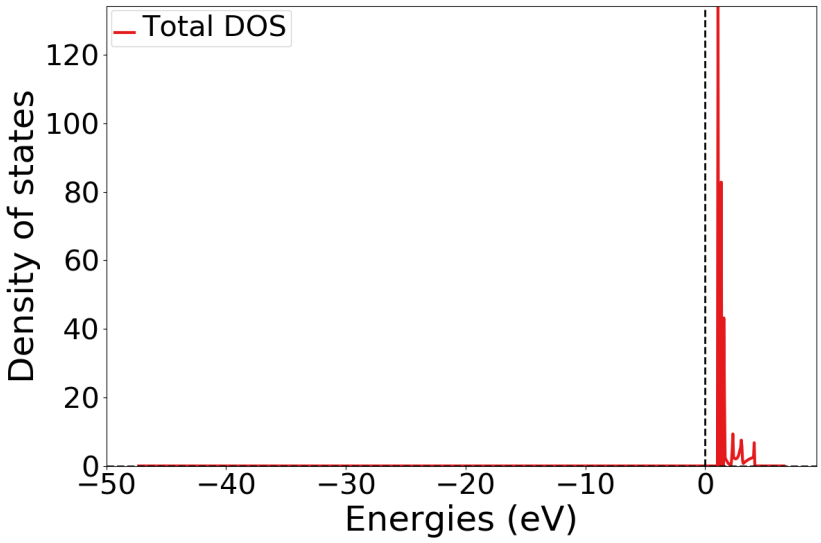
Figur 22: Charge density of Quinizarin with Yttrium for relaxed VASP calculation.



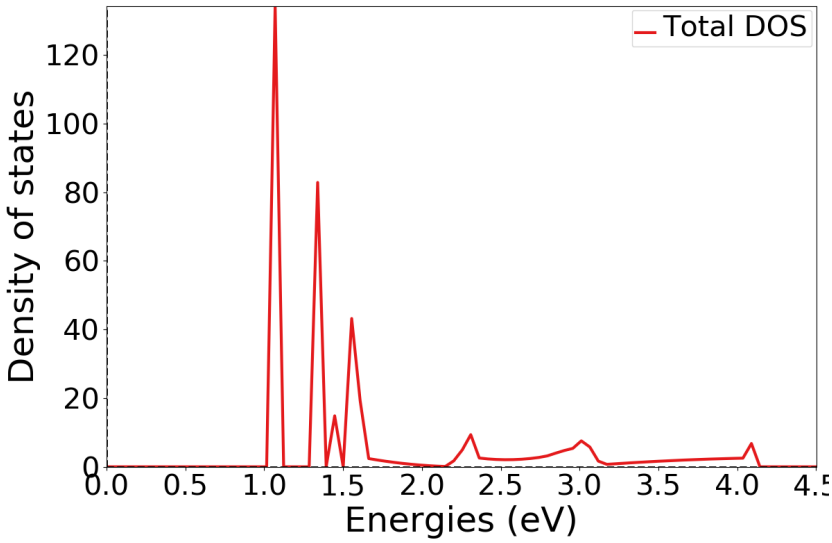
Figur 23: Structure of Quinizarin with Yttrium for static VASP calculation after relaxed calculation.



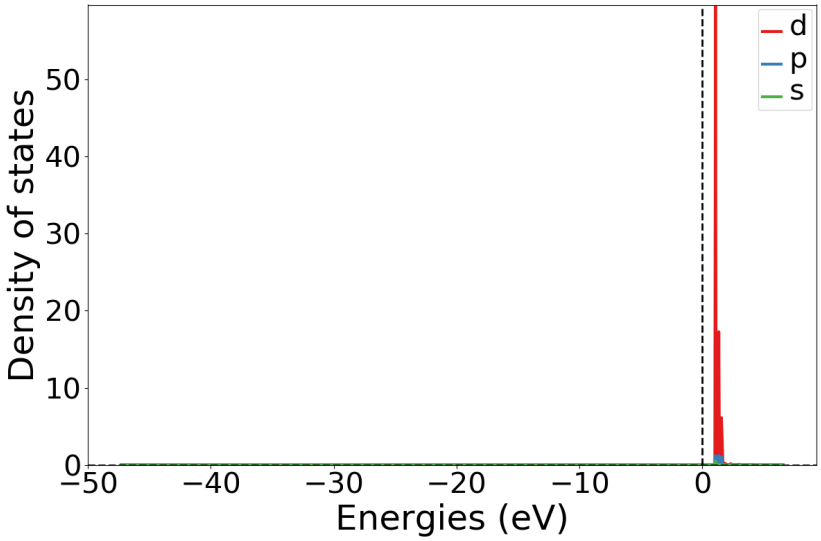
Figur 24: Charge density of Quinizarin with Yttrium for static VASP calculation after relaxed calculation.



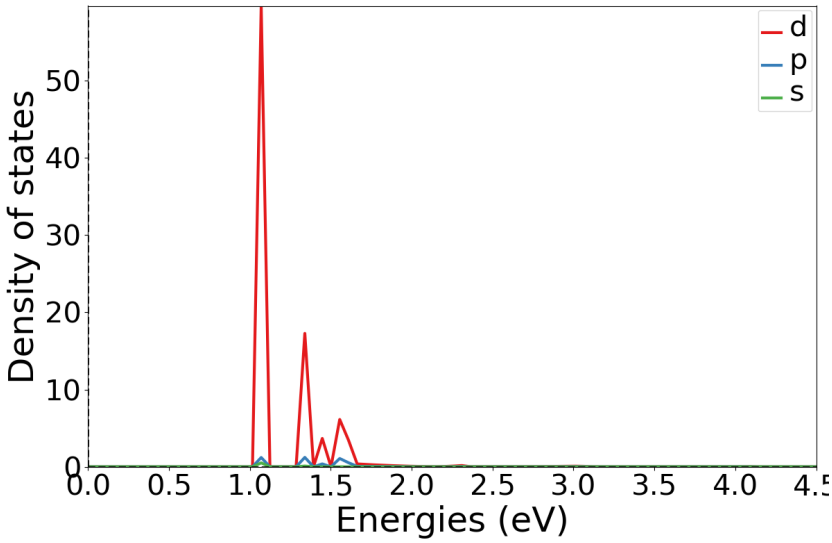
Figur 25: Plot of total DOS for Quinizarin with Yttrium.



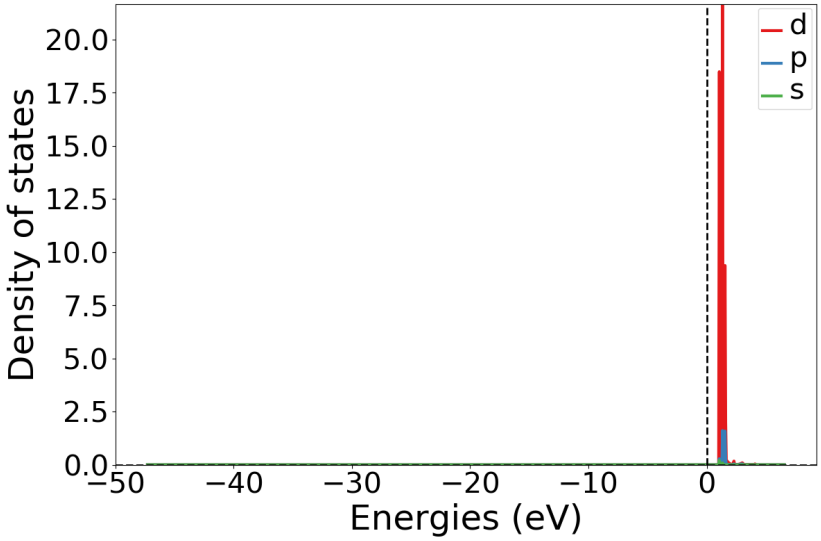
Figur 26: Plot of total DOS for Yttrium, zoomed in for energies between 0.0 eV and 4.5 eV.



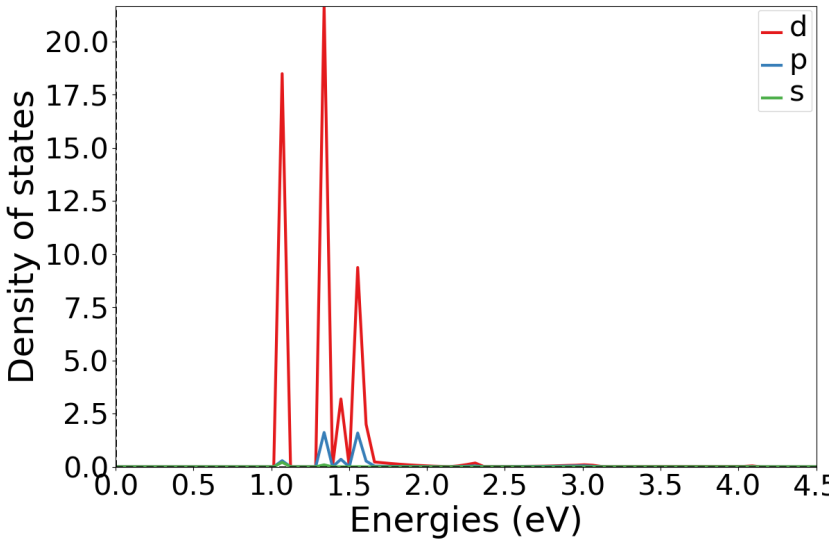
Figur 27: Plot of local DOS of atom number 25(Y in lower alcohol-group) for Quinizarin with Yttrium.



Figur 28: Plot of local DOS of atom number 25(Y in lower alcohol-group) for Quinizarin with Yttrium, zoomed in for energies between 0.0 eV and 4.5 eV.

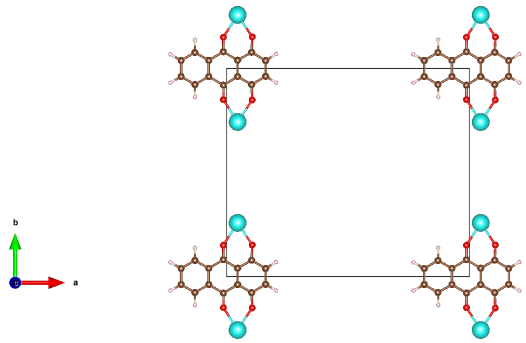


Figur 29: Plot of local DOS of atom number 26(Y in upper alcohol-group) for Quinizarin with Yttrium.

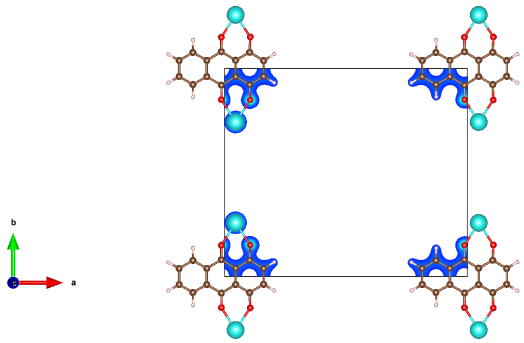


Figur 30: Plot of local DOS of atom number 26(Y in upper alcohol-group) for Quinizarin with Yttrium, zoomed in for energies between 0.0 eV and 4.5 eV.

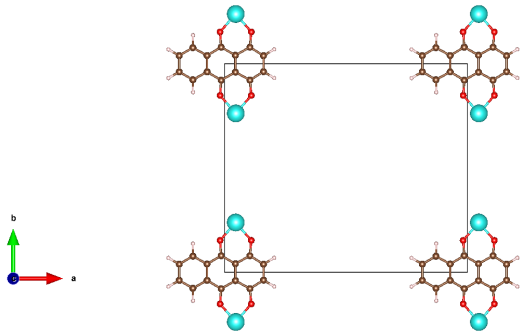
E Yb-bilder



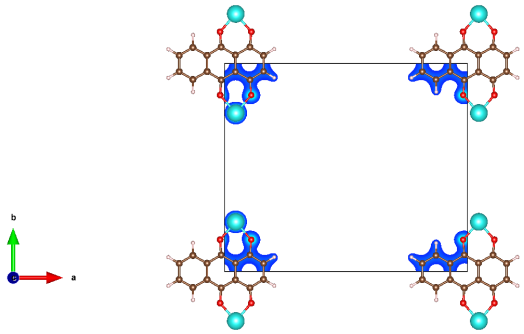
Figur 31: Structure of Quinizarin with Ytterbium for static VASP calculation.



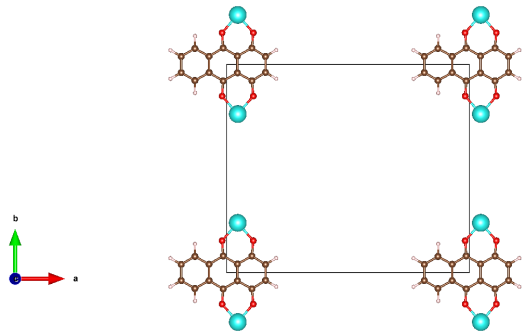
Figur 32: Charge density of Quinizarin with Ytterbium for static VASP calculation.



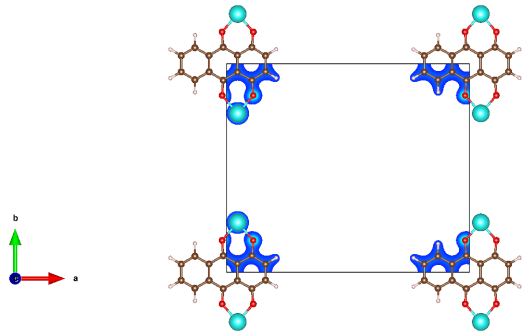
Figur 33: Structure of Quinizarin with Ytterbium for relaxed VASP calculation.



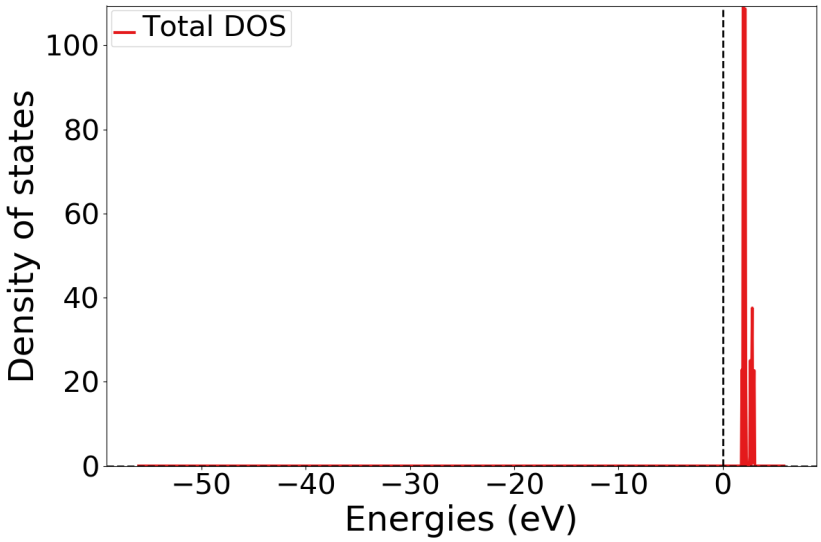
Figur 34: Charge density of Quinizarin with Ytterbium for relaxed VASP calculation.



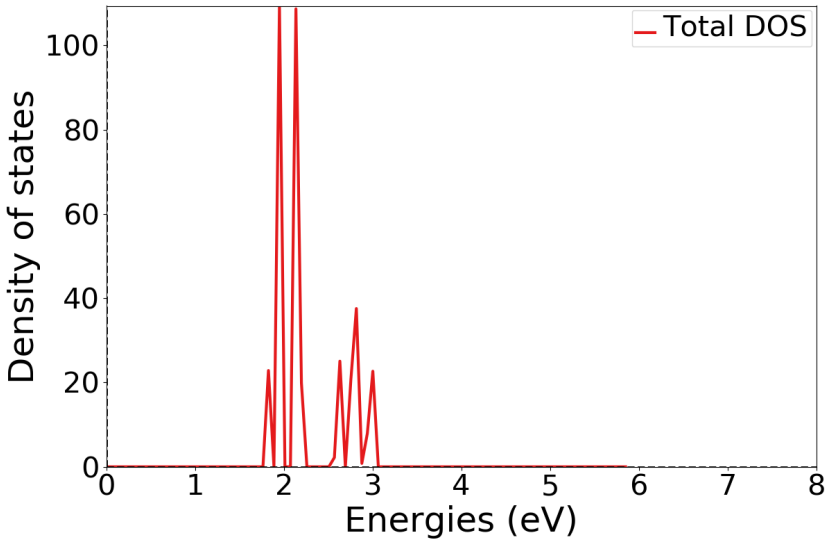
Figur 35: Structure of Quinizarin with Ytterbium for static VASP calculation after relaxed calculation.



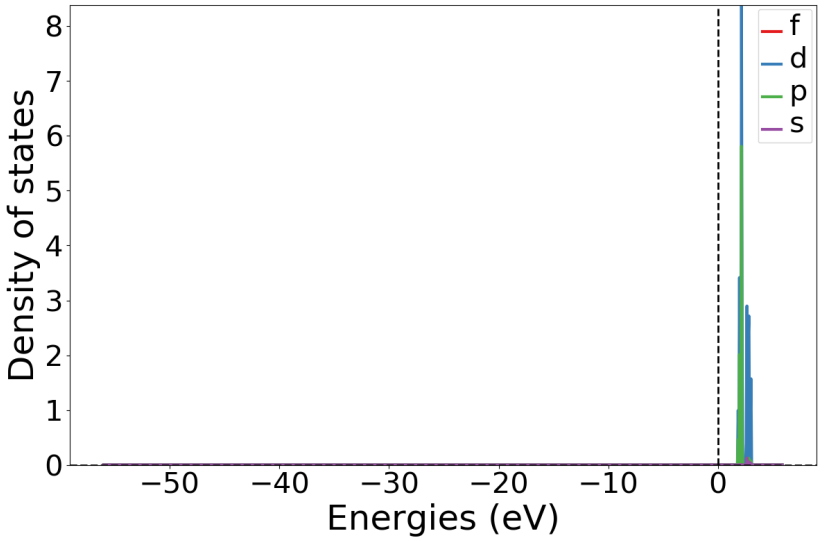
Figur 36: Charge density of Quinizarin with Ytterbium for static VASP calculation after relaxed calculation.



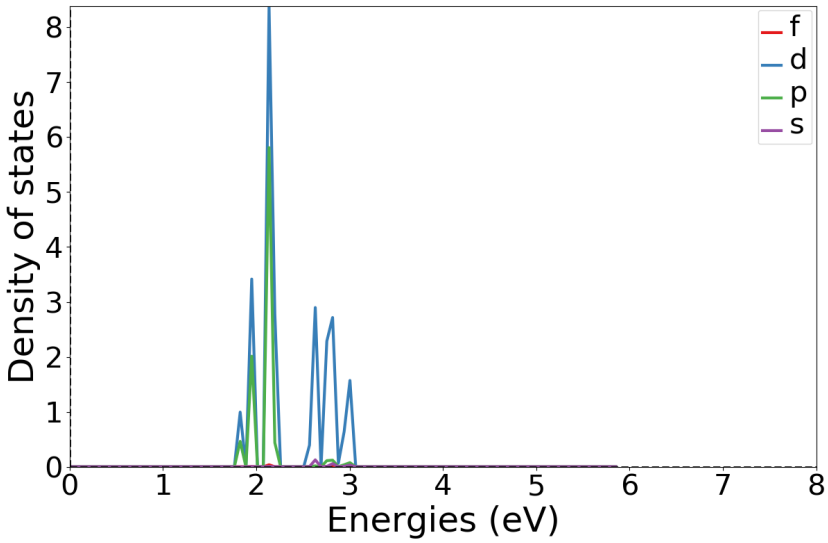
Figur 37: Plot of total DOS for Ytterbium.



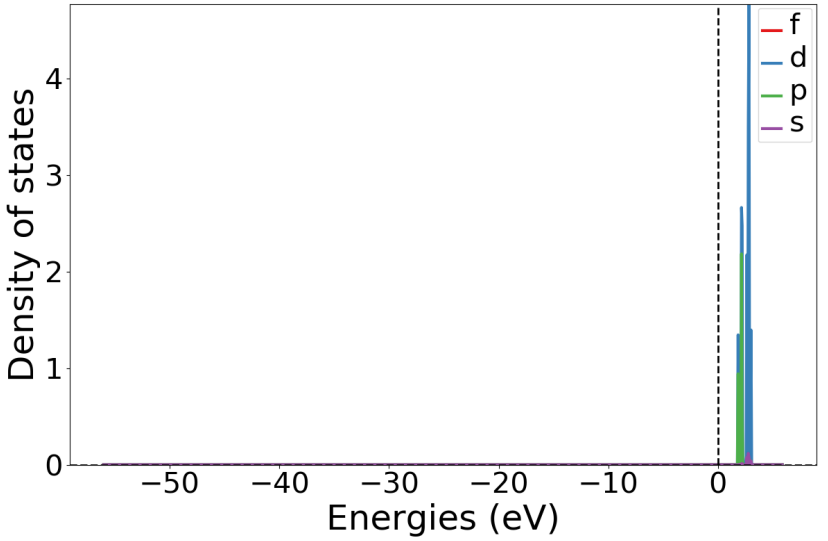
Figur 38: Plot of total DOS for Ytterbium, zoomed in for energies between 0.0 eV and 8.0 eV.



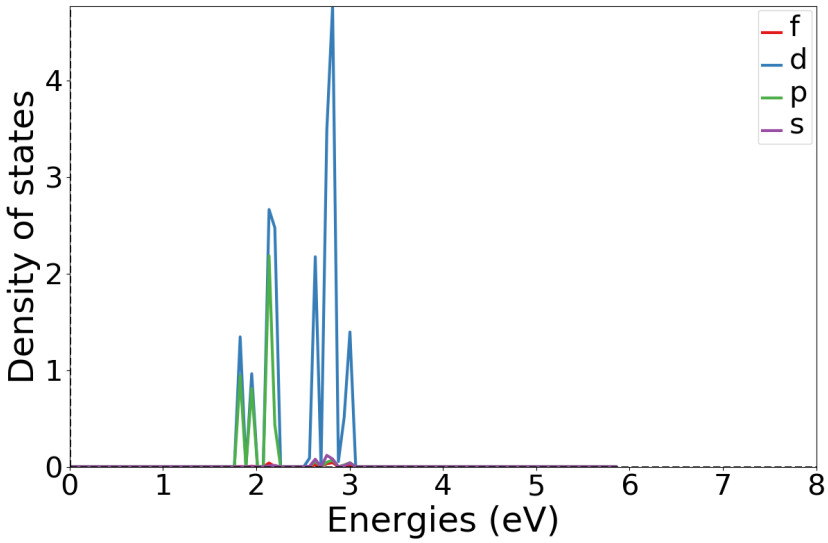
Figur 39: Plot of local DOS of atom number 25(Yb in lower alcohol-group) for Quinizarin with Ytterbium.



Figur 40: Plot of local DOS of atom number 25(Yb in lower alcohol-group) for Quinizarin with Ytterbium, zoomed in for energies between 0.0 eV and 8.0 eV.



Figur 41: Plot of local DOS of atom number 26(Yb in upper alcohol-group) for Quinizarin with Ytterbium.



Figur 42: Plot of local DOS of atom number 26(Yb in upper alcohol-group) for Quinizarin with Ytterbium, zoomed in for energies between 0.0 eV and 8.0 eV.

F Appendix 2