Project A20
FYS-MENA4111

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Week 44-

Abstract

Quinizarin can function as an organic sensetizer in an upconversion system. In ALD the organic molecule can possibly be deposited in a matrix of lanthanide flouride, to increase the efficiency of the upconversion process in the material. To see how this efficiency can increase and what energy levels can be absorbed by the material, it is wise to investigate the electronic band structure of the molecule. This paper will look in to Quinizarin's own electronic properties, as well as, Quinizarin with lanthanides replacing one a Hydrogen atom, to emulate Quinizarin inside the structure in a simple way.

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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.

- 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

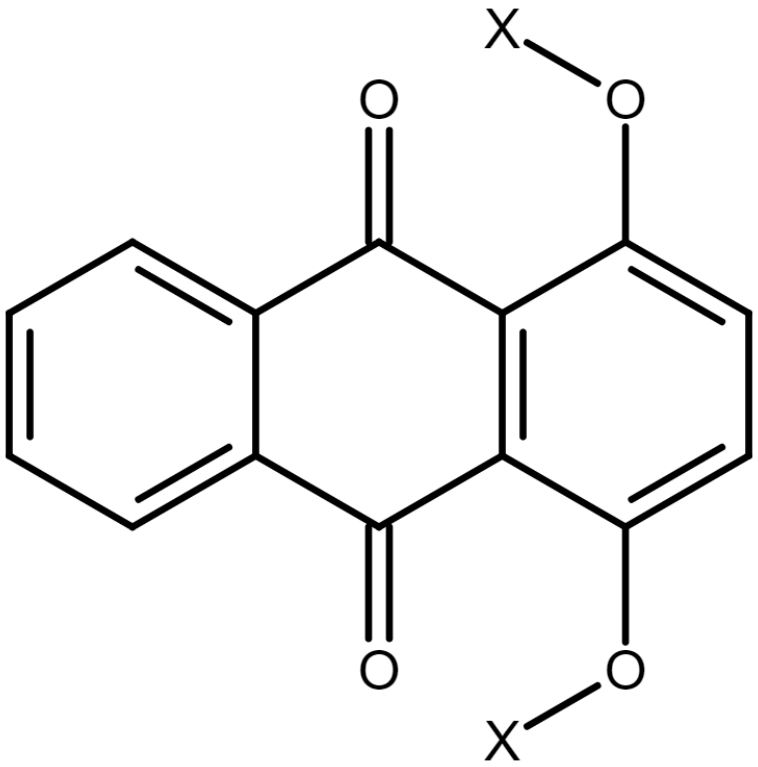
1 Introduction

Photons can be used for many things. However, not all photons are created equal. They come in many different energies, and not all energies are as simple to absorb. A way to increase the effieincy of photon-absorbing materials is by modifying it so that it can absorb photons with a low energy, collect that energy, and re-emit the photon with higher energy. This is known as up-conversion and has many uses. One use is to increase the efficiency of solar panels by allowing it to collect more of the sunlight, where the up-conversion system can be a thin-film on the top of the panel. A different use is to increase the energy to the point where the emitted photon can become ionizing and work as a bacteria or virus killer.

Up-conversion is a phenomenon where incoming photons are re-emitted with a higher energy than they entered with. The photons excite electrons in a material, and by conduction of those electrons they can move to other atoms, where they are further excited. The electron ends up in a high energy state and de-excites releasing all the energy. However, the process can be very inefficient due to narrow energy bands in the material. A form of increasing this efficiency is by adding a material with a wide energy band to allow absorption of photons with more varied energy.

This paper will focus on an organic compound known as Quinizarin. The compound is an organic dye and has a broad energy band. This means it can absorb a broad spectrum of photons energies. The excited electrons from this energy band can move to the actual up-conversion system and hereby increase the efficiency of the up-conversion. The planned up-conversion system will consist of Quinizarin as an organic sensitizer, Nd+3 and Yb+3 as electron migrators (transporting the electrons to the site of de-exitation), and Tm+3 as accumulator and activator (collecting excited electrons and upconverting them, and de-exitation site for said electrons). The system is planned to be inserted into a matrix of YbF3 or possibly YF3.

Since Quinizarin is such an important piece of the system it is wise to know how it interacts with the other materials. This study will therefore investigate how Quinizarin's electronic band structure changes when the Hydrogen in the alcohol group is replaced with different atoms. In this case: Yb, Nd, Tm and Y. See figure 1 for an illustration.



Figur 1: Molecular structure of Quinizarin with H in -OH replaced with atom X. X can be H, Y, Yb, Nd or Tm. Structure drawn with online illustrator from Chem-Space.

2 Method

"Briefly about the method; choice of parameters, cutoff, etc."

2.1 Convergence

Testing for convergence of energy and k-point is important to determine if the variables in INCAR or KPOINTS is good enough to be used for further calculations, mostly to ensure good and applicable results. A good convergence should give an error of less than $1 \cdot 10^{-3}$.
The testing of convergence is done by performing VASP calculations with different values of either energy-cutoff (ENCUT) or k-point density.
Energy: ENCUT: 300 to 900
K-point: K-point density: 1.0 to 6.0

2.2 Static

2.3 Relax

2.4 Static after relax

2.5 DOS

3 Results

3.1 Energy convergence

Started to convergence around 450 eV for ENCUT.

3.2 K-points convergence

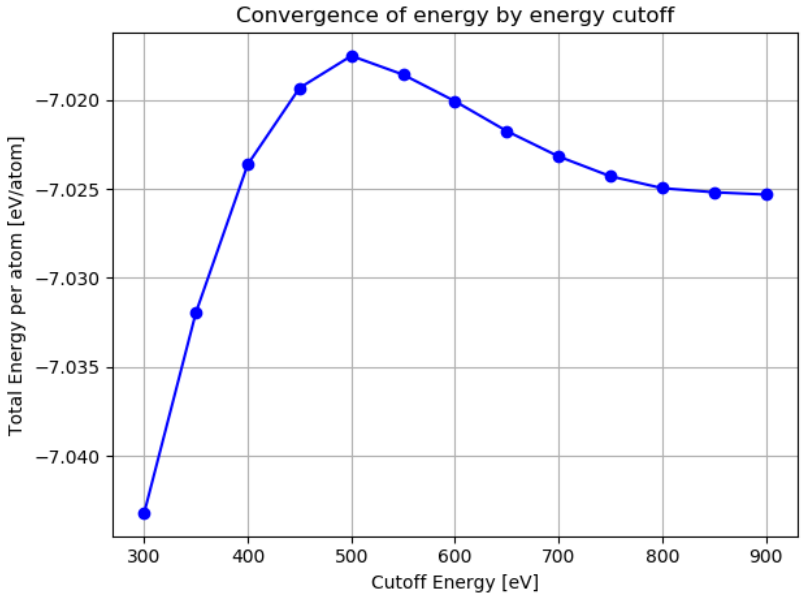
4 Discussion

5 Conclusion

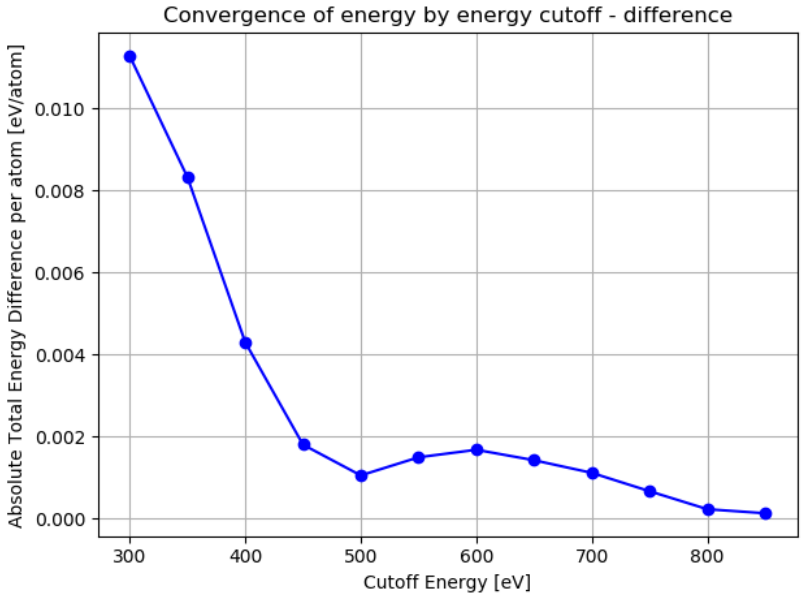
6 References

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

A Convergence energy

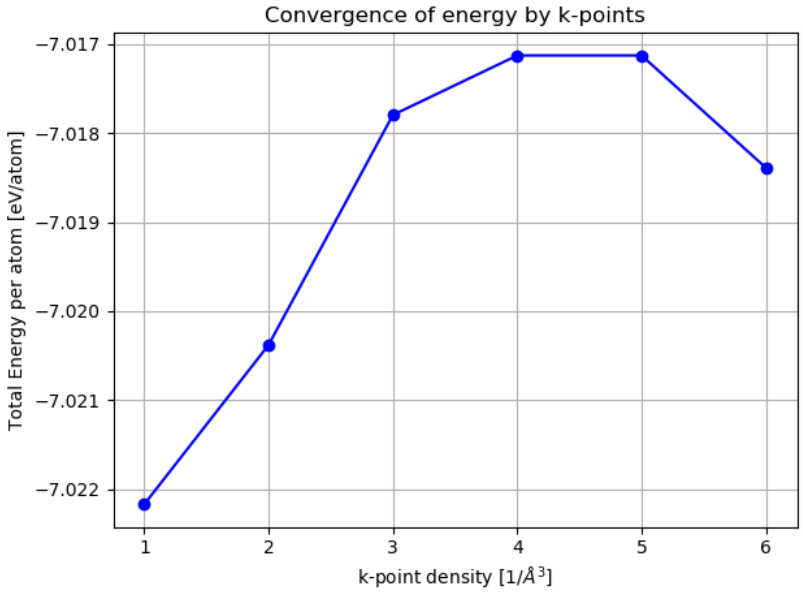


Figur 2: Plot of energy convergence for Quinizarin, with ENCUT ranging from 300 eV to 900 eV.

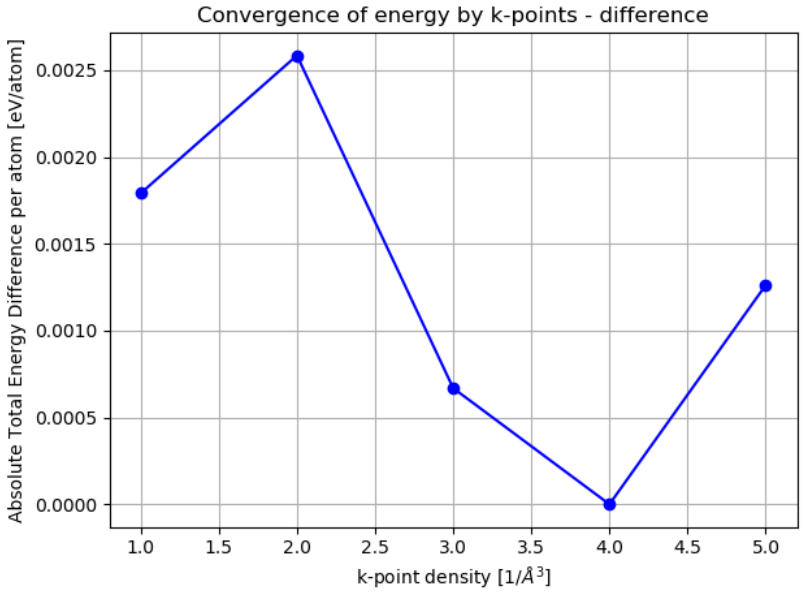


Figur 3: Plot of the difference in energy convergence for Quinizarin, given by ENCUT.

B Convergence k-points

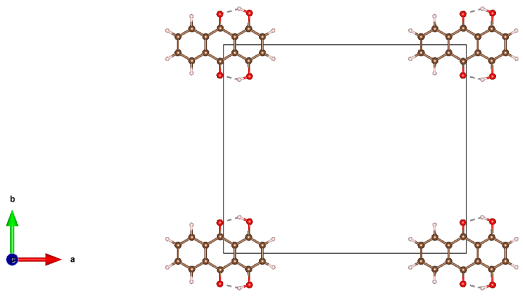


Figur 4: Plot of energy convergence for Quinizarin, with k-point density ranging from 1 to 6.

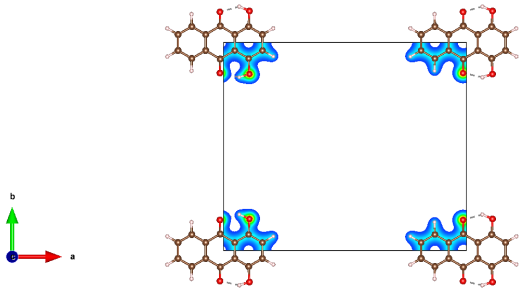


Figur 5: Plot of the difference in energy convergence for Quinizarin, given by k-point density.

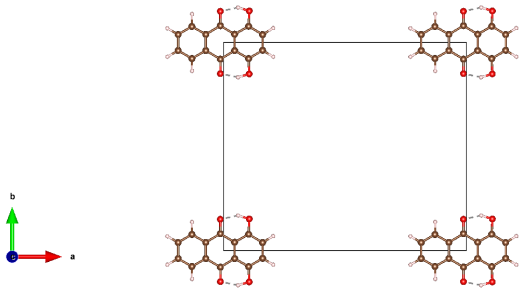
C Quinizarin-bilder



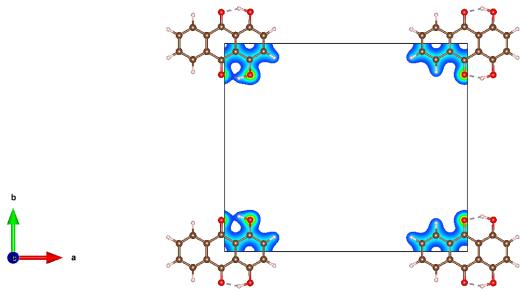
Figur 6: Structure of Quinizarin for static VASP calculation.



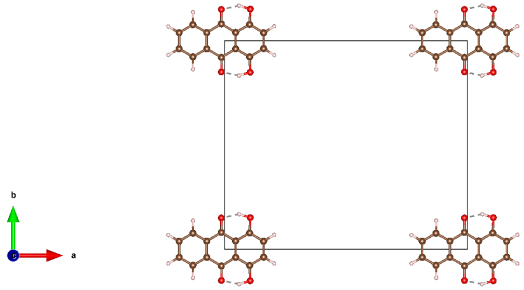
Figur 7: Charge density of Quinizarin for static VASP calculation.



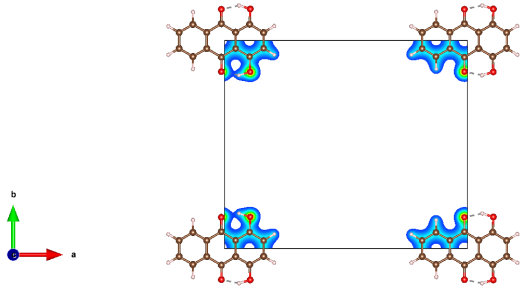
Figur 8: Structure of Quinizarin for relaxed VASP calculation.



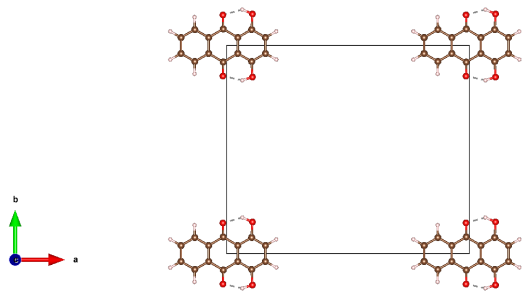
Figur 9: Charge density of Quinizarin for relaxed VASP calculation.



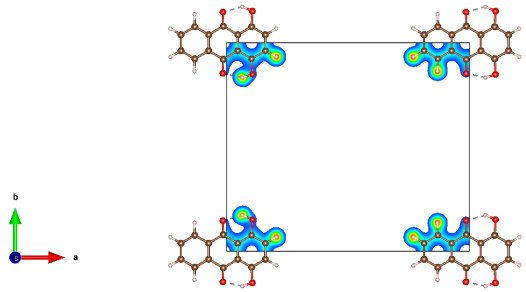
Figur 10: Structure of Quinizarin for static VASP calculation after relaxed calculation.



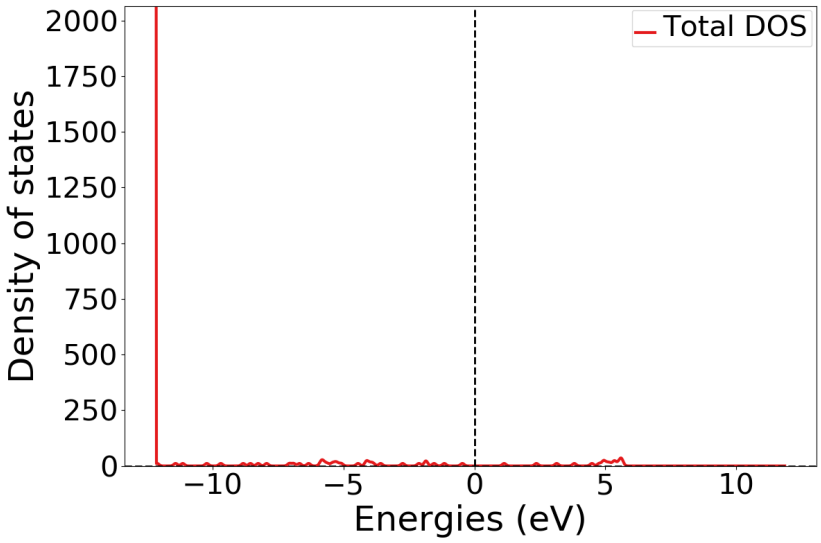
Figur 11: Charge density of Quinizarin for static VASP calculation after relaxed calculation.



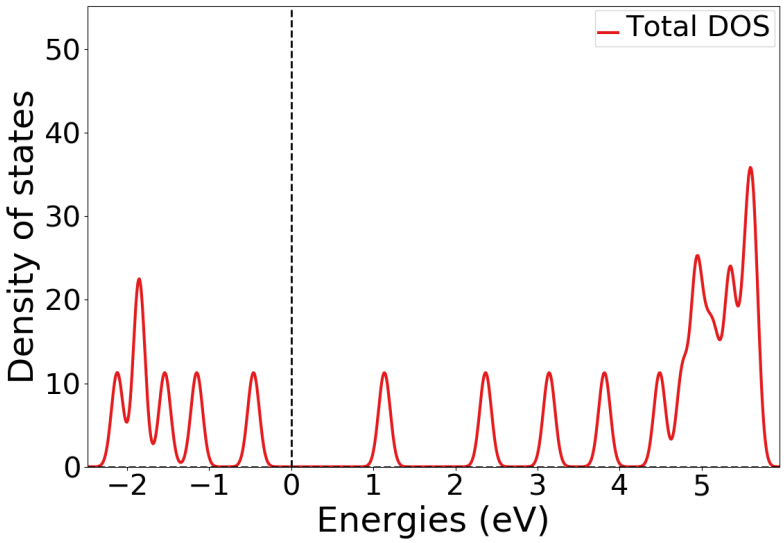
Figur 12: Structure of Quinizarin for DOS VASP calculation.



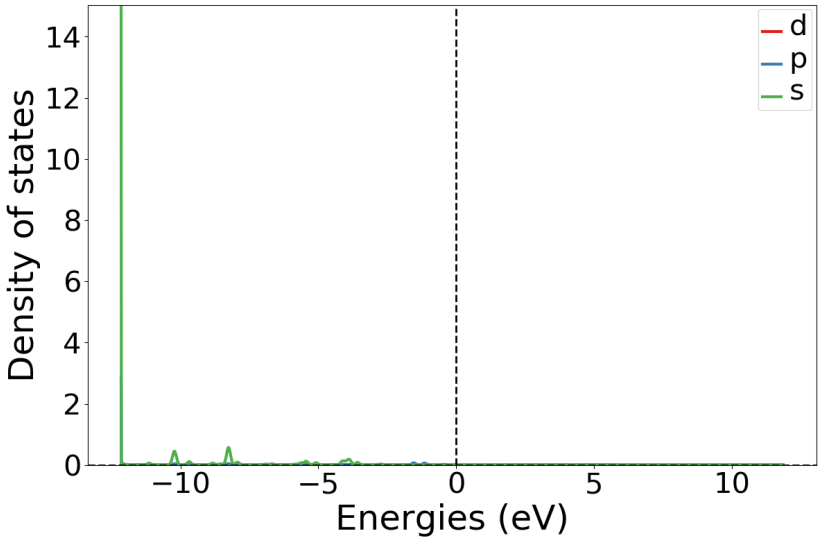
Figur 13: Charge density of Quinizarin for DOS VASP calculation.



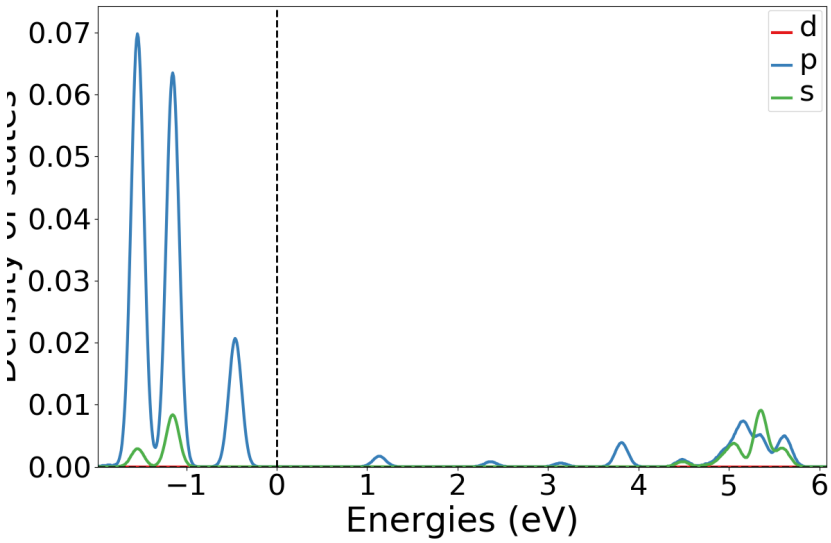
Figur 14: Plot of total DOS for Quinizarin.



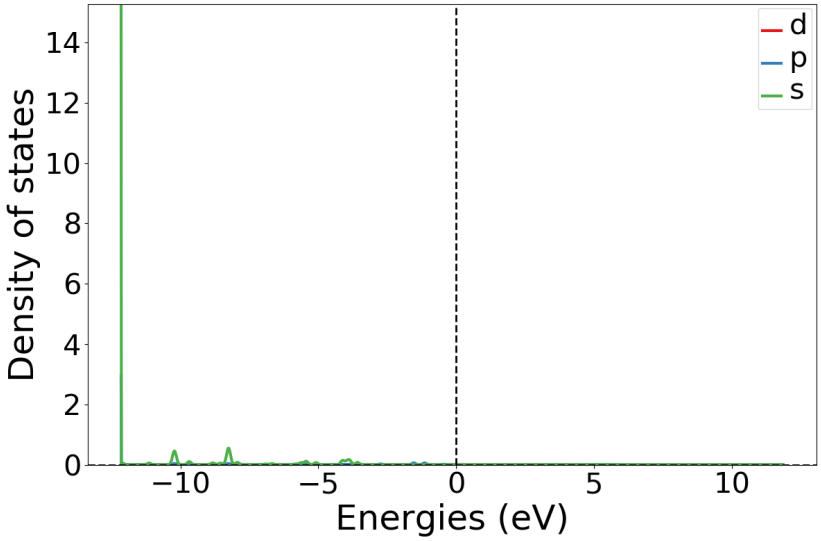
Figur 15: Plot of total DOS for Quinizarin, zoomed in for energies between 4.0 eV and 8.0 eV.



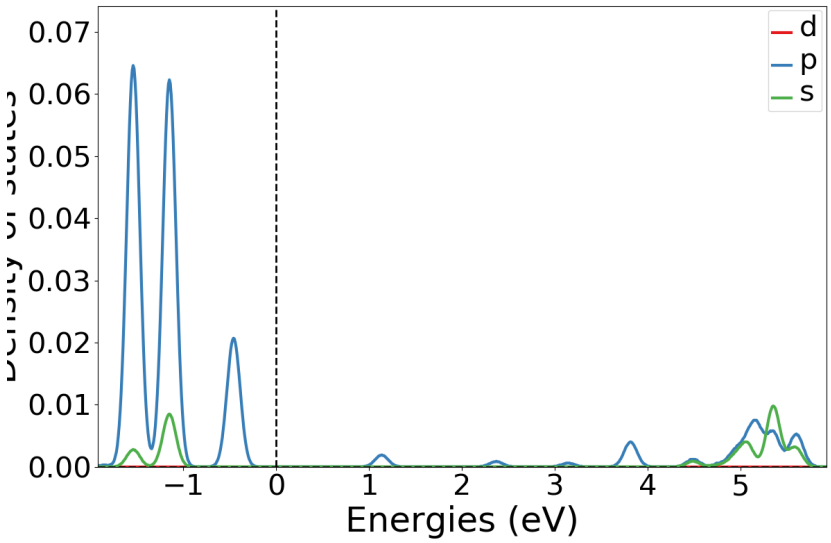
Figur 16: Plot of local DOS for atom number 25(H in alcohol-group) for Quinizarin.



Figur 17: 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.

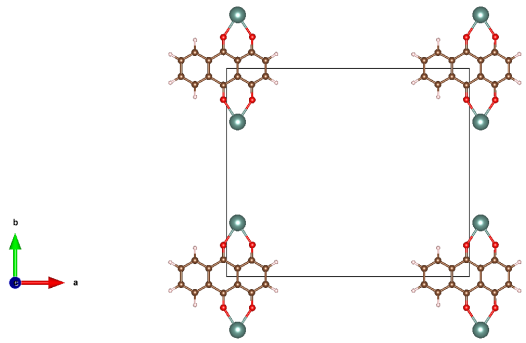


Figur 18: Plot of local DOS for atom number 26(H in alcohol-group) for Quinizarin.

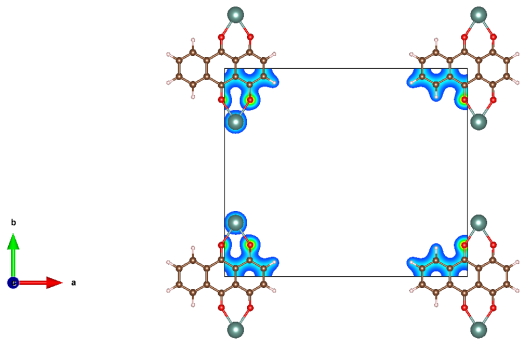


Figur 19: Plot of local DOS for atom number 26(H in alcohol-group) for Quinizarin, zoomed in for energies between 4.0 eV and 8.0 eV.

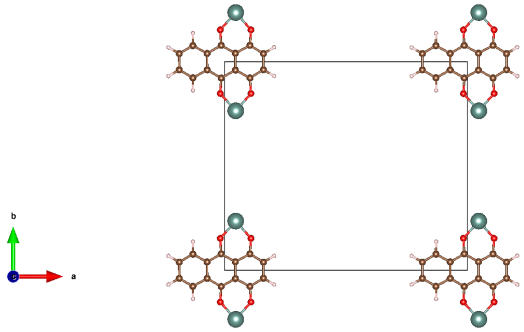
D Y-bilder



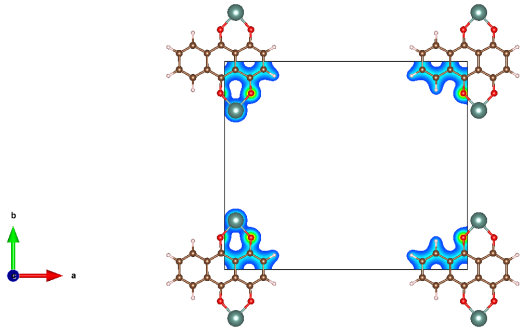
Figur 20: Structure of Quinizarin with Yttrium for static VASP calculation.



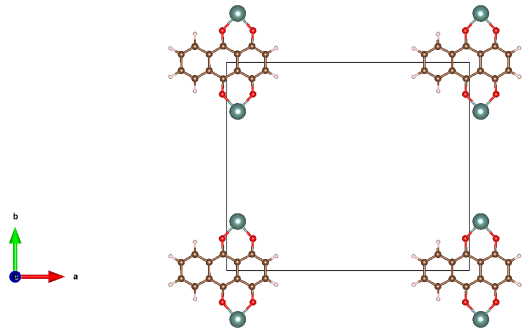
Figur 21: Charge density of Quinizarin with Yttrium for static VASP calculation.



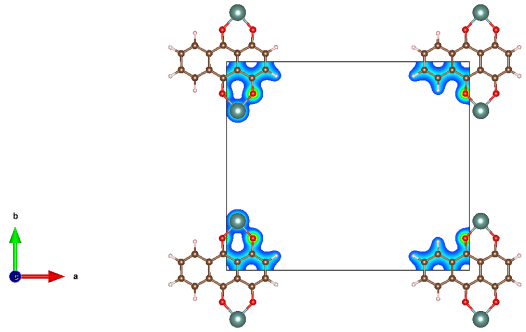
Figur 22: Structure of Quinizarin with Yttrium for relaxed VASP calculation.



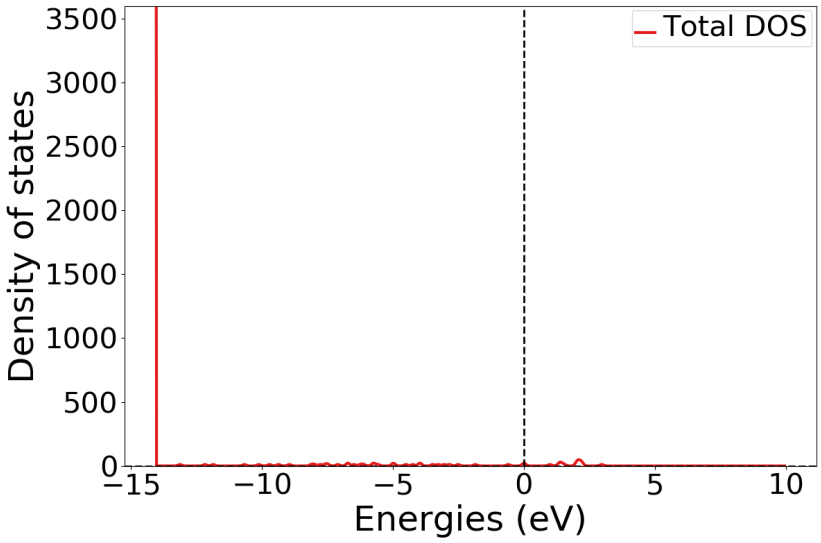
Figur 23: Charge density of Quinizarin with Yttrium for relaxed VASP calculation.



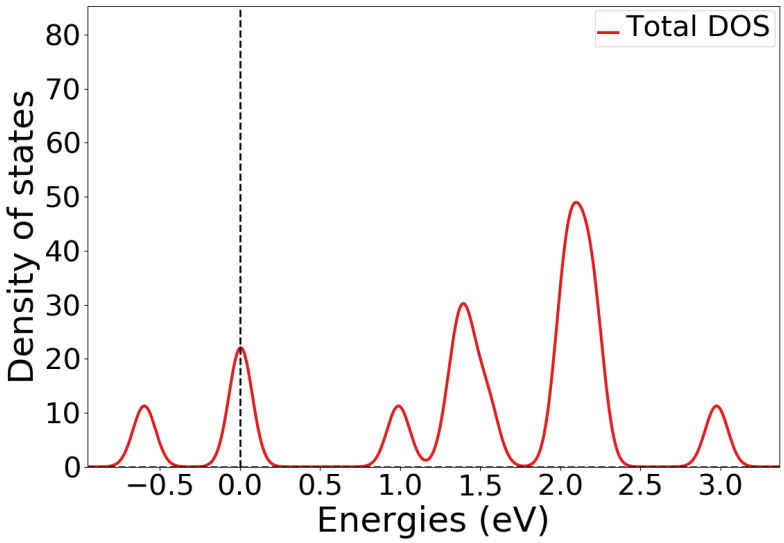
Figur 24: Structure of Quinizarin with Yttrium for static VASP calculation after relaxed calculation.



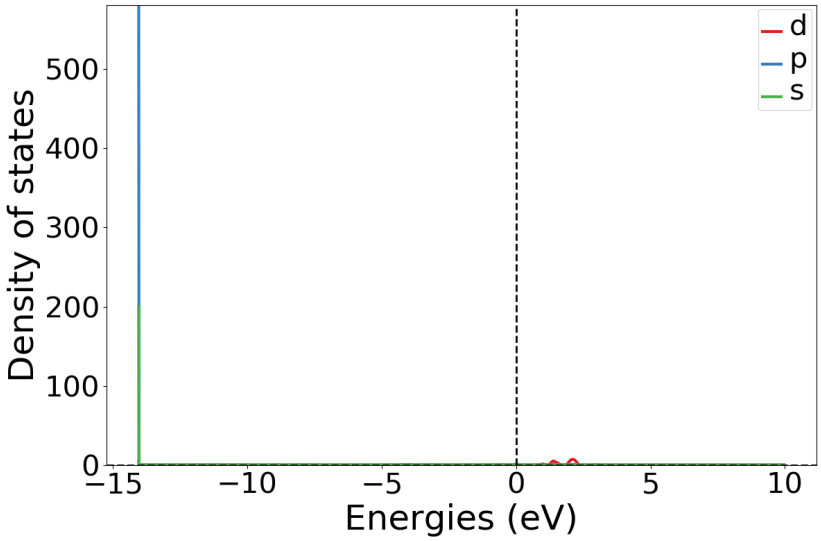
Figur 25: Charge density of Quinizarin with Yttrium for static VASP calculation after relaxed calculation.



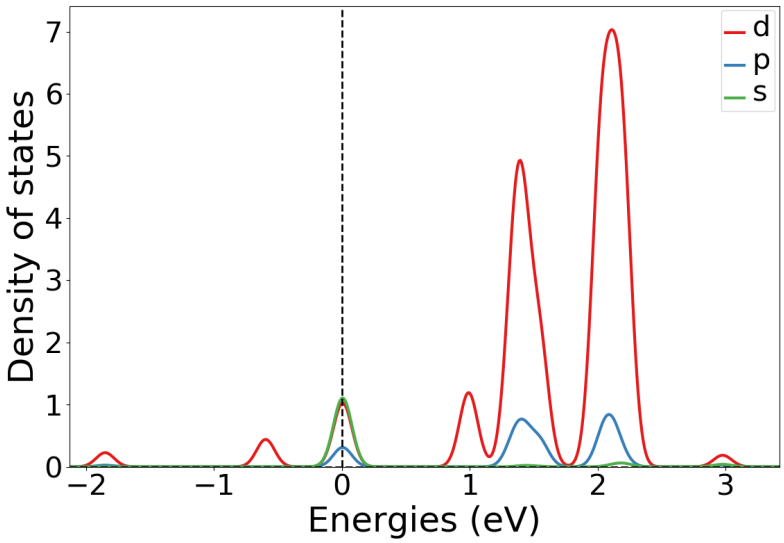
Figur 26: Plot of total DOS for Quinizarin with Yttrium.



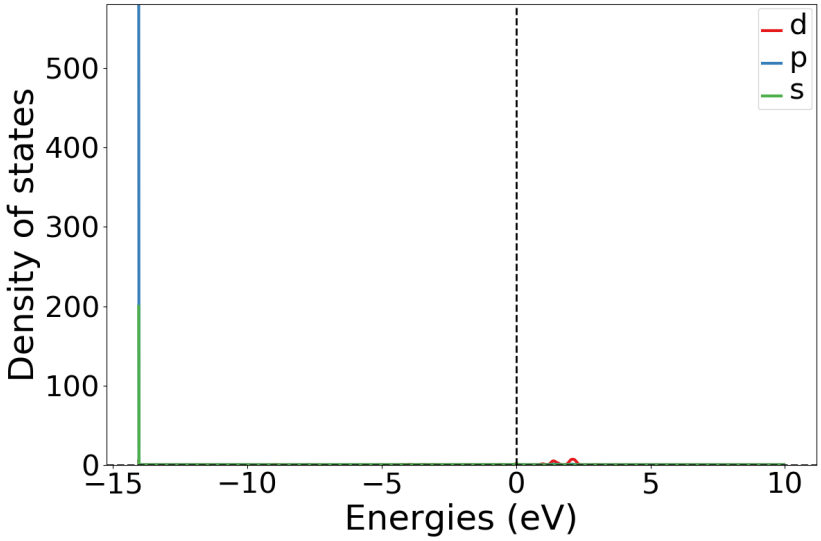
Figur 27: Plot of total DOS for Yttrium, zoomed in for energies between 0.0 eV and 4.5 eV.



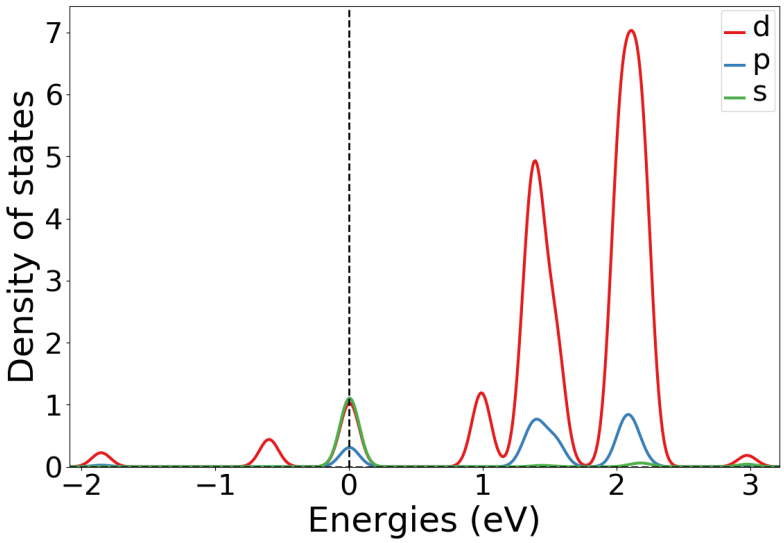
Figur 28: Plot of local DOS of atom number 25(Y in lower alcohol-group) for Quinizarin with Yttrium.



Figur 29: 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.

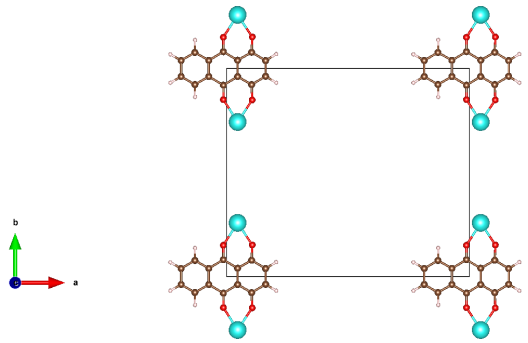


Figur 30: Plot of local DOS of atom number 26(Y in upper alcohol-group) for Quinizarin with Yttrium.

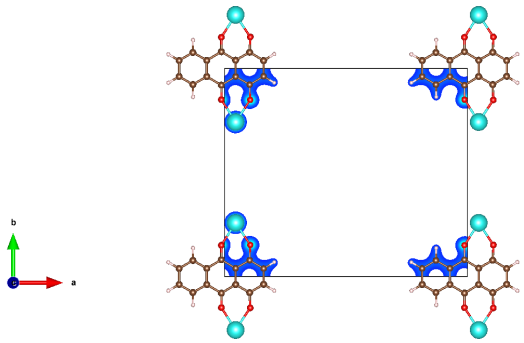


Figur 31: Plot of local DOS of atom number 26(Y in upper alcohol-group) for Quinizarin with Yttrium, zoomed in for energies between 0.0 eV and 4.5 eV.

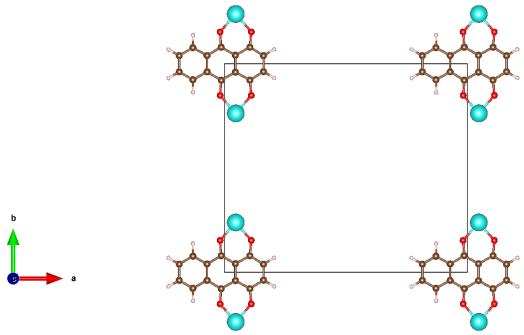
E Yb-bilder



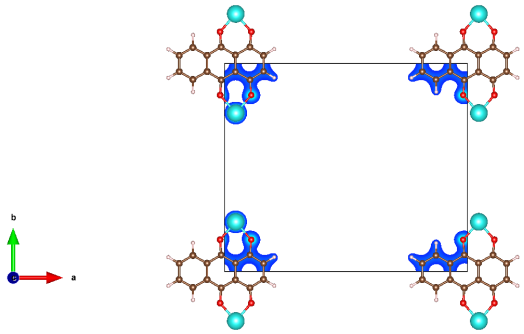
Figur 32: Structure of Quinizarin with Ytterbium for static VASP calculation.



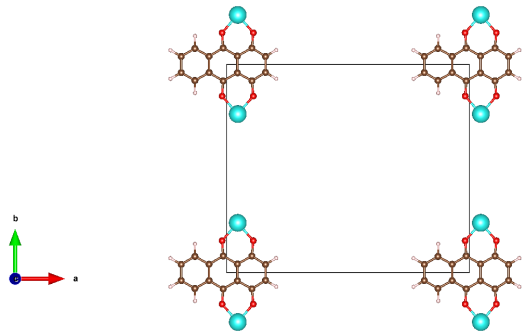
Figur 33: Charge density of Quinizarin with Ytterbium for static VASP calculation.



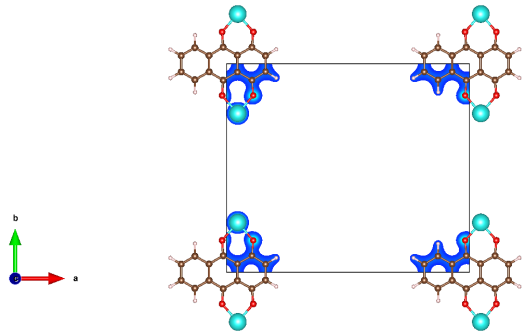
Figur 34: Structure of Quinizarin with Ytterbium for relaxed VASP calculation.



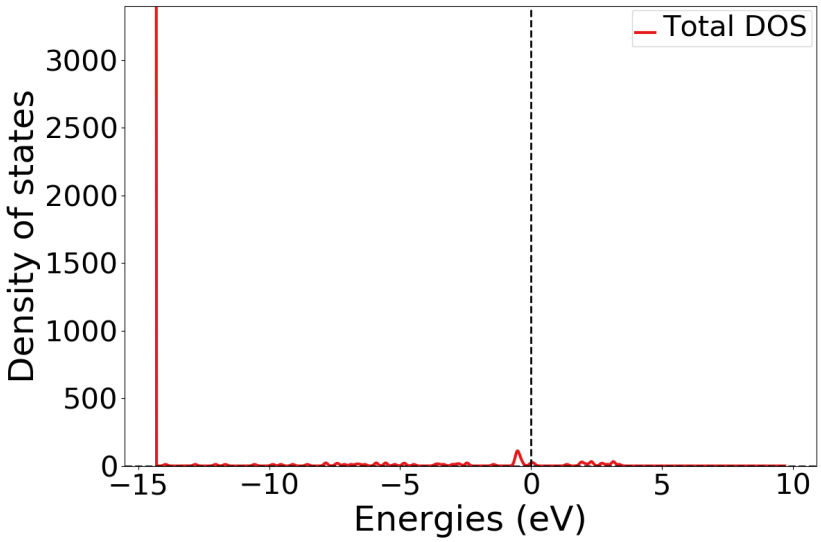
Figur 35: Charge density of Quinizarin with Ytterbium for relaxed VASP calculation.



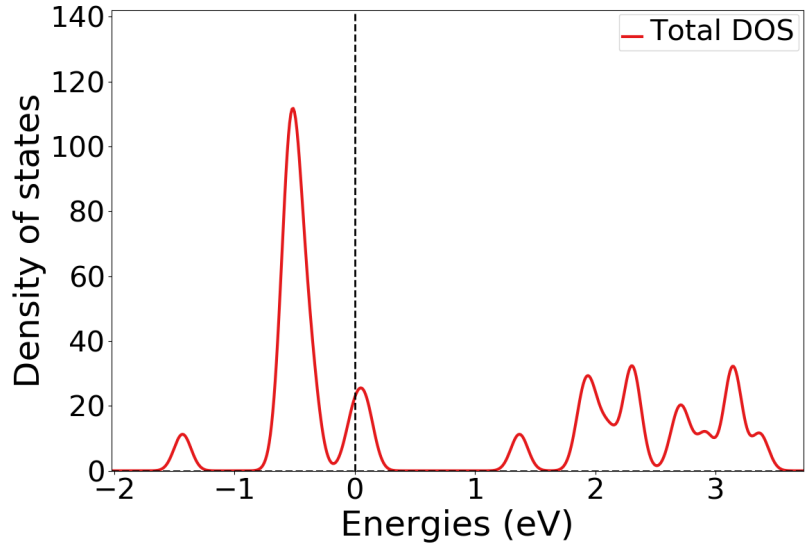
Figur 36: Structure of Quinizarin with Ytterbium for static VASP calculation after relaxed calculation.



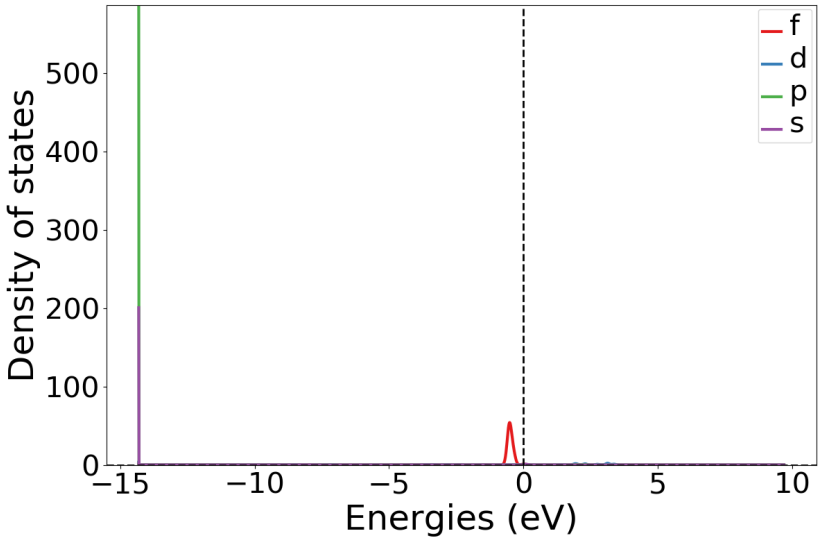
Figur 37: Charge density of Quinizarin with Ytterbium for static VASP calculation after relaxed calculation.



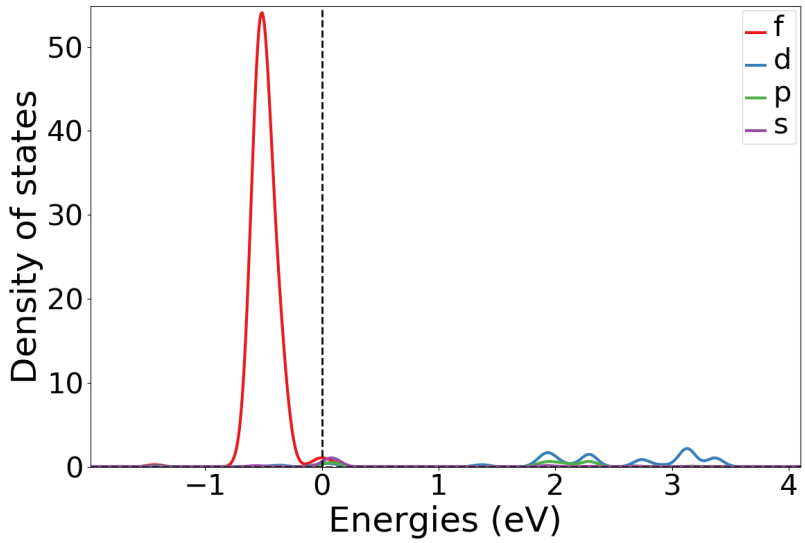
Figur 38: Plot of total DOS for Ytterbium.



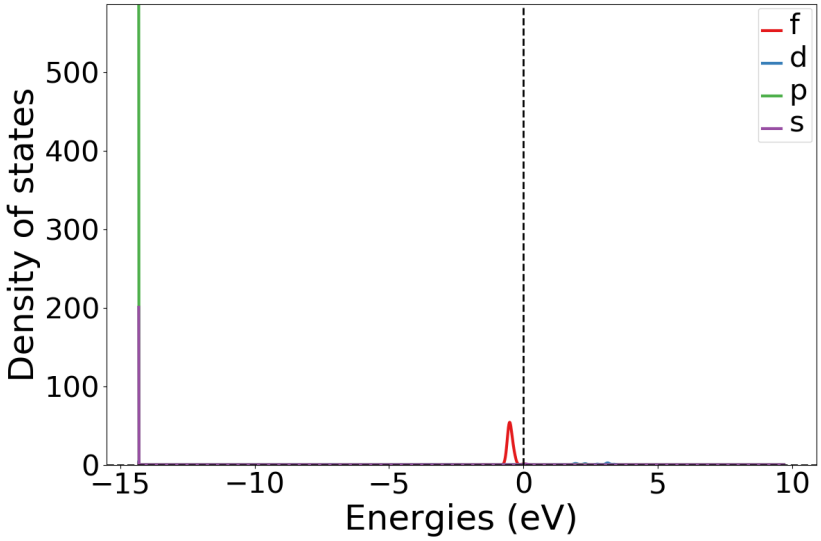
Figur 39: Plot of total DOS for Ytterbium, zoomed in for energies between 0.0 eV and 8.0 eV.



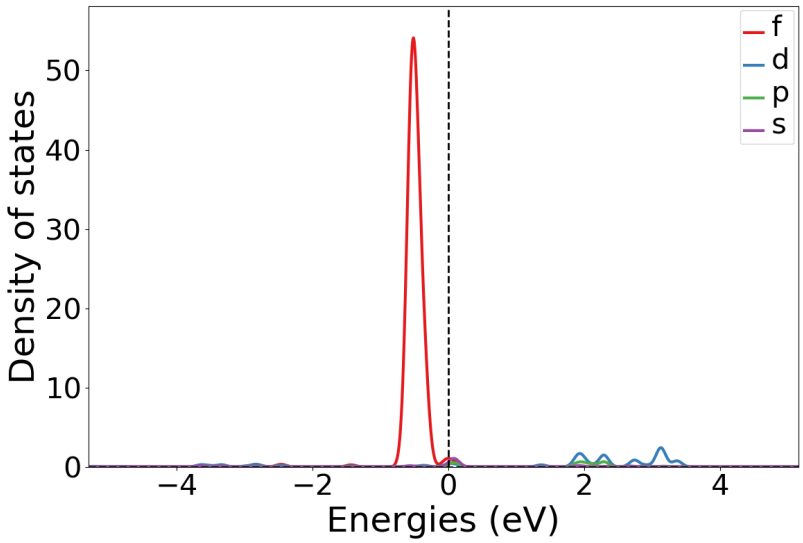
Figur 40: Plot of local DOS of atom number 25(Yb in lower alcohol-group) for Quinizarin with Ytterbium.



Figur 41: 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 42: Plot of local DOS of atom number 26(Yb in upper alcohol-group) for Quinizarin with Ytterbium.



Figur 43: 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