UCLouvain
École polytechnique de Louvain

LMAPR2451
Atomistic and nanoscopic simulations

Study of the optical properties of Pyrite (FeS_2)
Preliminary results

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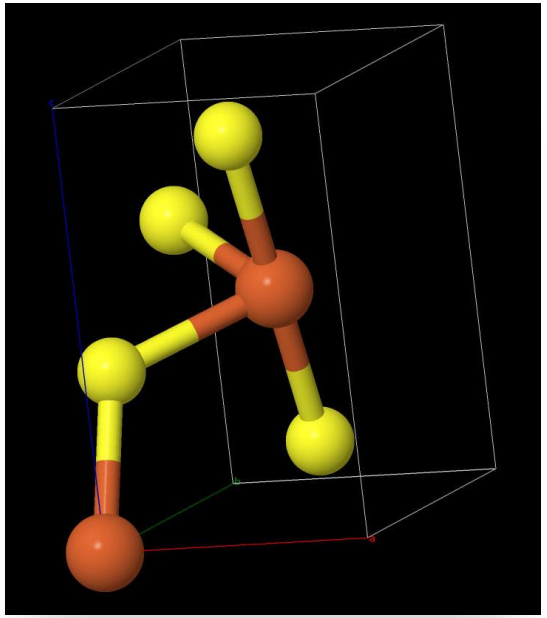
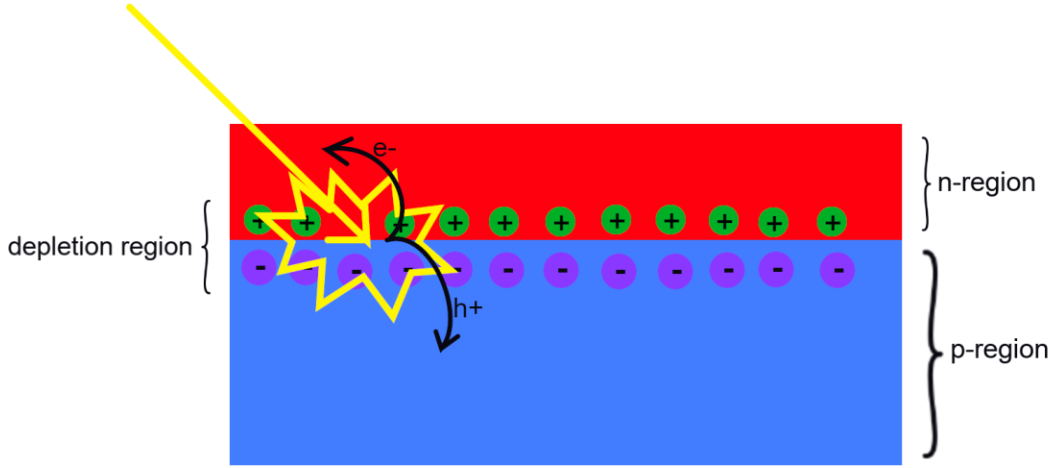
Representation of FeS_2 in Abinit

mp-1522

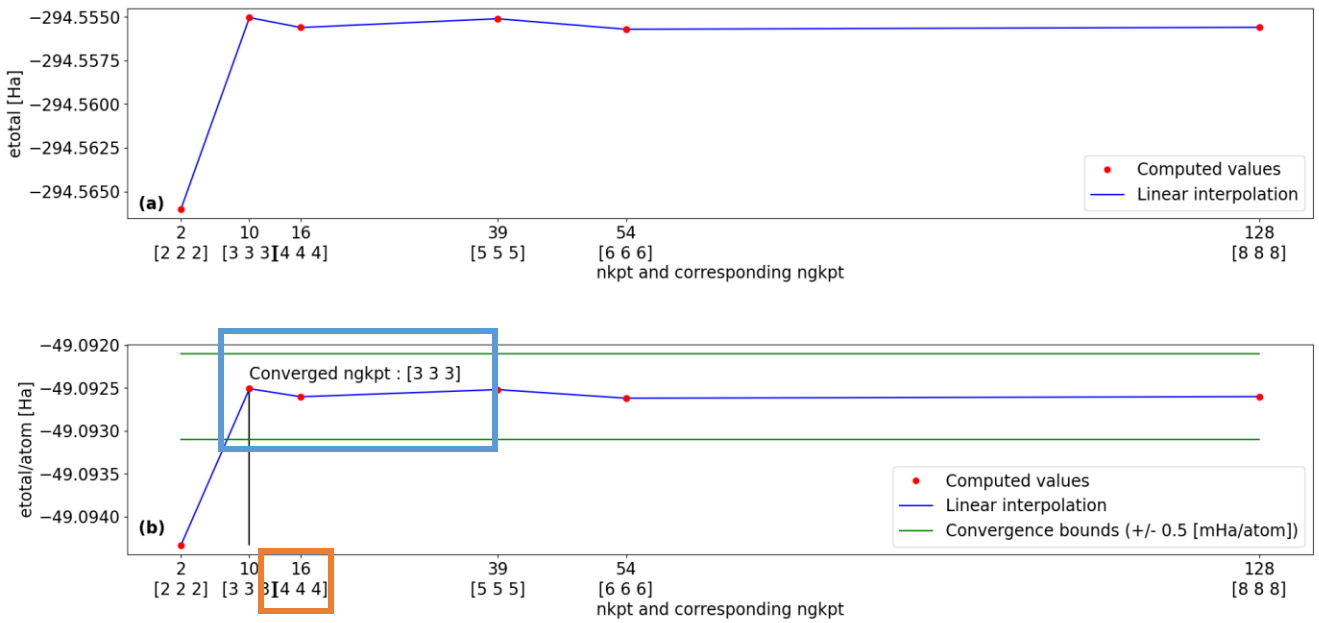
```
acell    3.390 4.438 5.411 Angstr # to be converged (ecut & ngkpt)
ntypat   2

znucl    26 16
natom    6
typat    1 1 2 2 2 2
xred     0       0       0
         0.5     0.5     0.5
         0       0.206   0.3753
         0       0.794   0.6247
         0.5     0.294   0.8753
         0.5     0.706   0.1247
```



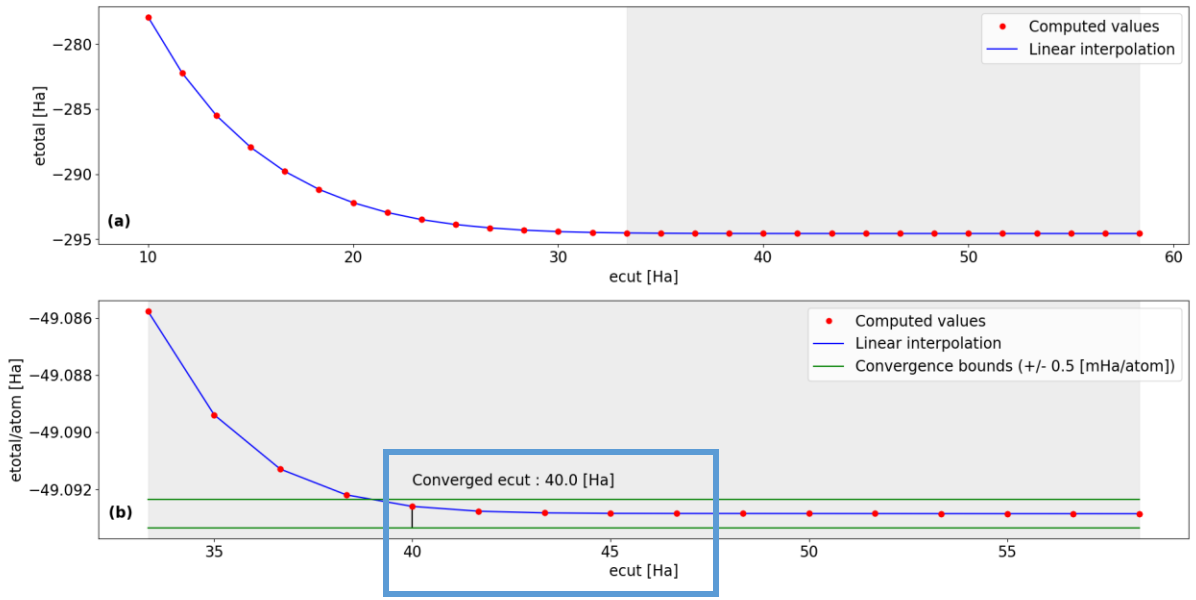


Convergence studies

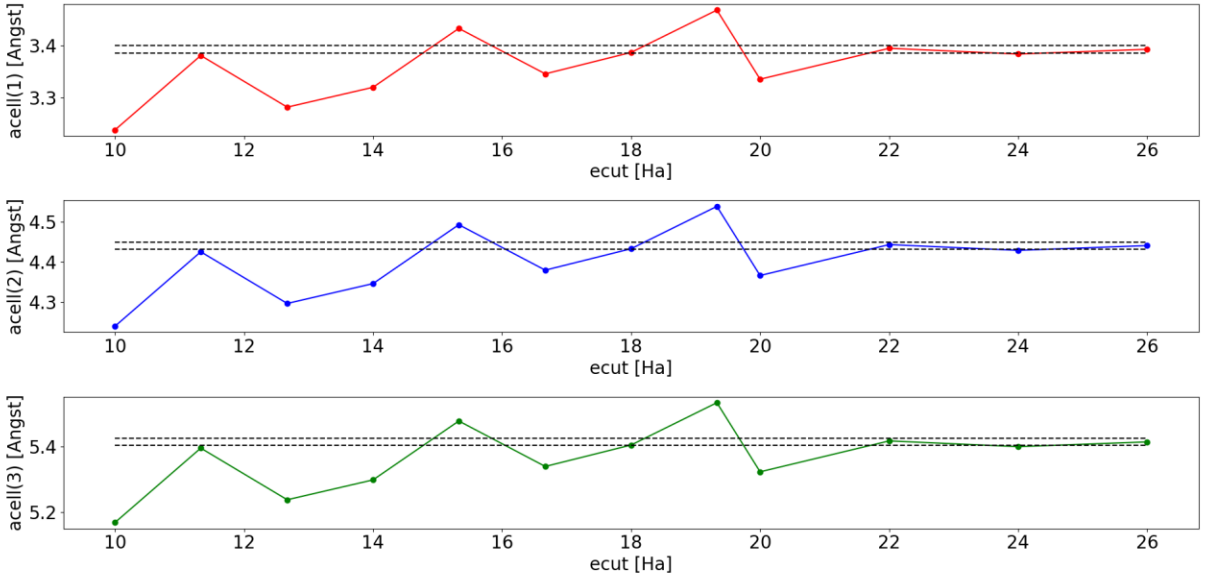


Total energy/atom with respect to `ngkpt`

Total energy/atom with respect to `ecut`



Convergence studies



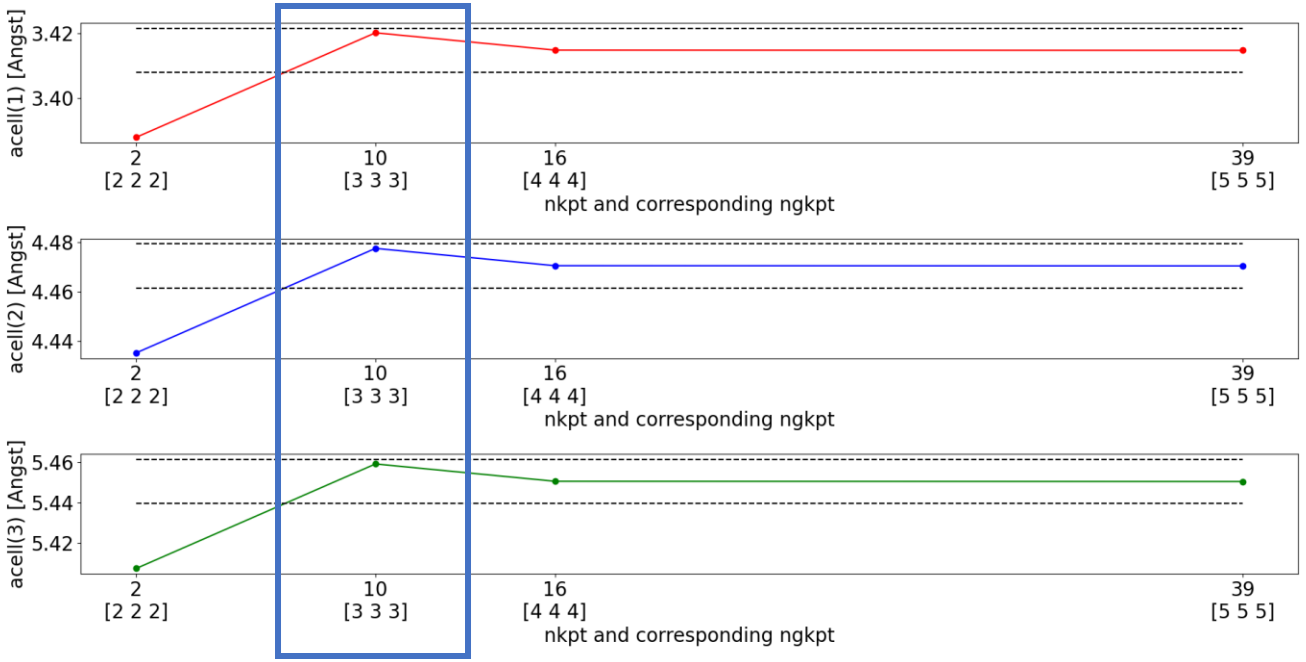
`acell` with respect to `ecut`

up to `ecut` = `50` [Ha]

To be completed...

`acell` with respect to `ngkpt`

up to `nkpt` = `128` (`ngkpt` = `[8 8 8]`)



(Further) Optical studies

1) Band structure + band gap

- Using the converged values
- => frequency range of absorbed light (optical modes)

2) Optics

- Using `optic, RPA` approximation
- => Frequency-dependant linear dielectric tensor
- => Absorption coefficient

3) Excitonic analysis

- Bethe-Salpeter calculations
- => Absorption spectra including excitonic effects