Project 5 FYS4150

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Abstract

To do:
Write file every temp

Contents

1 Introduction

MD: "Numerical method for studying many-particle systems such as molecules, clusters, and even macroscopic systems such as gases, liquids and solids "

Kjetils notater: Simulere bevegelse N atomer og molekyler basert på klassisk newtonsk dynamikk: $F_i = m\frac{\mathrm{d}ri}{\mathrm{d}t} = -\frac{\partial U}{\partial r:i}$. Kraften er ofte sterkt avstandsavhengig og kan komme fra eks. Lennard Jones potensial. [1].

Fysikk:

Material science: Can use potentials dervied from non-relativistic Schrödinger equation to investigate lattic and defect dynamics at atomistic scale. [2]

Kjemi: behavoiur ideal gas, chemical reacton $A+A \rightarrow B+B$ with hard sphere potential and Lennard Jones potential, [3]

Bio: Simulate membranes Molecular dynamics—the science of simulating the motions of a system of particles—applied to biological macromolecules gives the fluctuations in the relative positions of the atoms in a protein or in DNA as a function of time. Knowledge of these motions provides insights into biological phenomena such as the role of flexibility in ligand binding and the rapid solvation of the electron transfer state in photosynthesis. Molecular dynamics is also being used to determine protein structures from NMR [4]

God link til "hva er MD": https://udel.edu/ arthij/MD.pdf

2 Theory

Discuss why the velocity of atoms are given from Maxwell-Boltzmann distrubution. - nonzero net momentum.

3 Method

Describe briefly each class and its general purpose: System

atom

io unitconverter vec3 VelocityVerlet LennardJones random.h statisticssampler

flow chart(s?)

4 Result

1 unitcell:

Bandgap (med ismear = -5) 0.4342 28 2.1177 2.5519 2.0 0.0

Ferminivå: """ grep fermi OUTCAR ISMEAR = -5; SIGMA = 0.10 broadening in eV -4-tet -1-fermi 0-gaus E-fermi : 2.1202 """

Bandstruktur: M -gamma -R -X -Gamma

5 O2

Ecut converged for $\frac{\Delta E}{\Delta E_{Cutoff}} = \frac{750eV}{50eV}$

6 Supercells:

6.1 Bandstructure

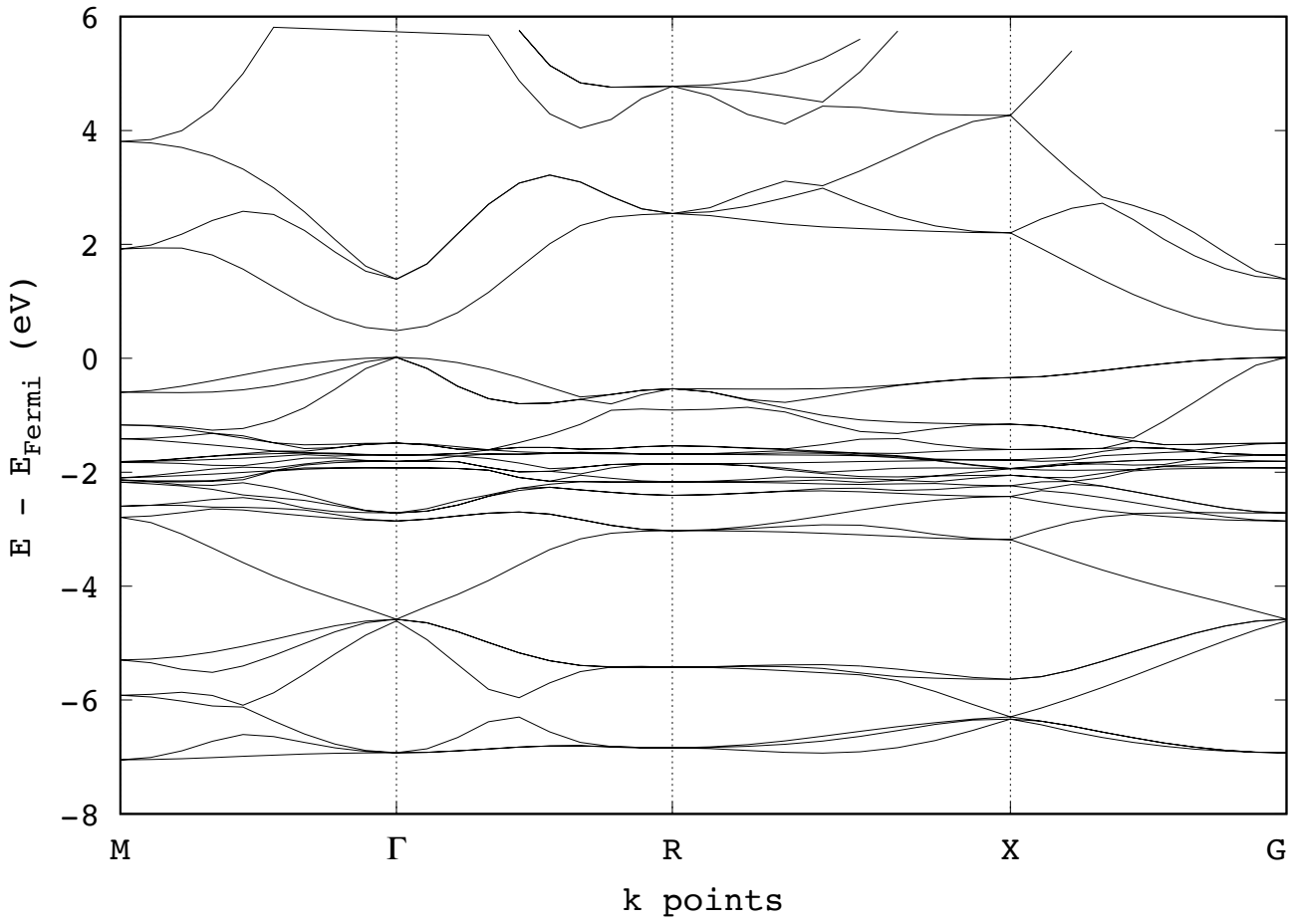


Figure 6.1

6.2 Energy, force and pressure

relaxed energies:

Table 6.1: $3 * 3 * 3$

Supercell size	MxForce	Pressure	TOTEN
$1 \times 1 \times 1$, without defect	0.000	-0.2600	-27.194124
$1 \times 1 \times 1$, with defect			
$2 \times 2 \times 2$	0.040	-0.3800	-210.664202
$3 \times 3 \times 3$	0.023	0.2800	-727.495258
$4 \times 4 \times 4$	0.033	-0.2200	-1734.014857

To do: Look at energy per atom - OBS: Oxygen

6.3 Bandgap and electronic structure

VBM occ: 2 for alle, CB-occ = 2 for alle!

Table 6.2: Bandgaps

System	Gap	Band nr	VBM	CBM
L=1, no defect	0.4342	28	2.1177	2.5519
L=2	0.7951	221	2.155	2.9501
L=3	0.5323	753	2.1478	2.6801
L=4	0.4767	1789	2.1474	2.6241

6.4 DOS

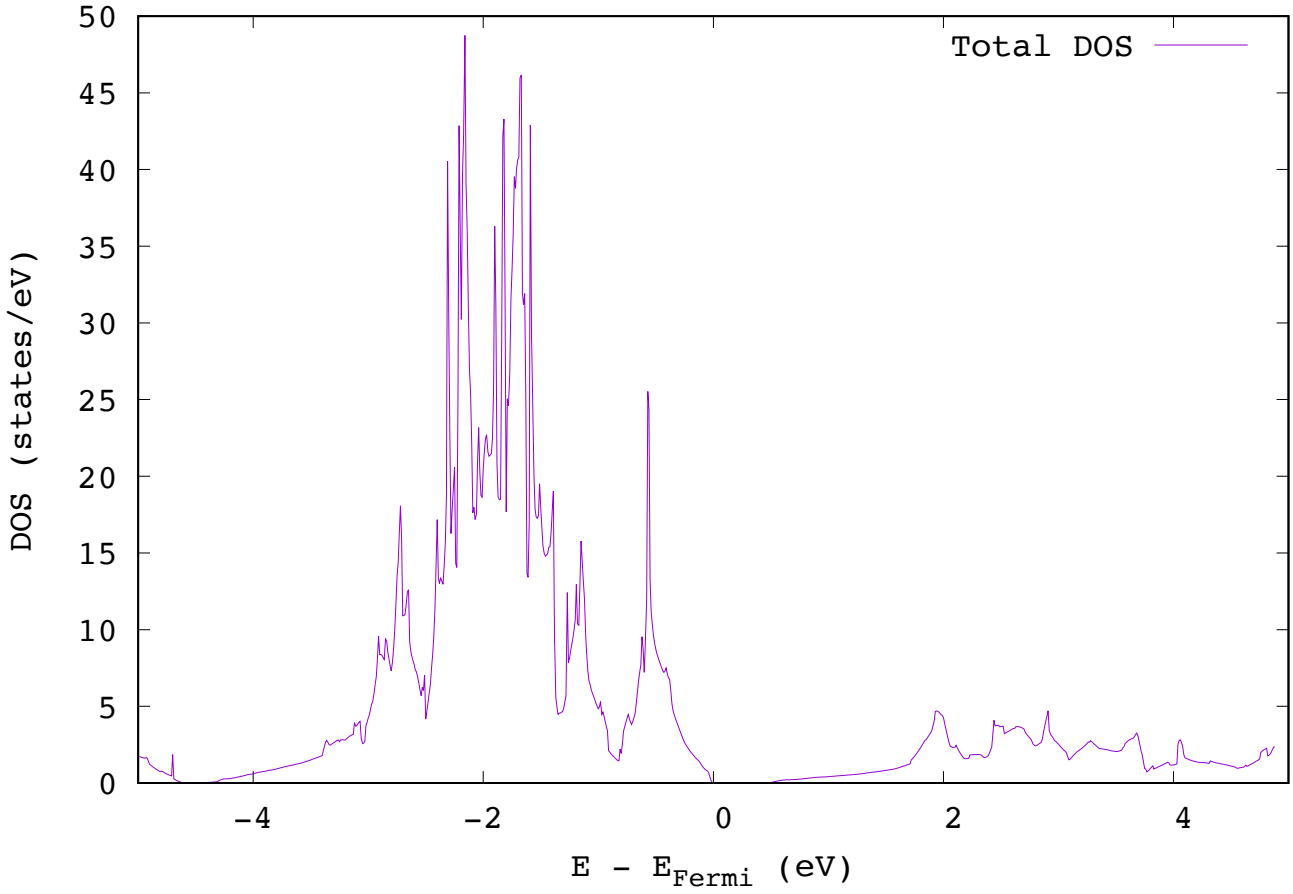


Figure 6.2: DOS for the

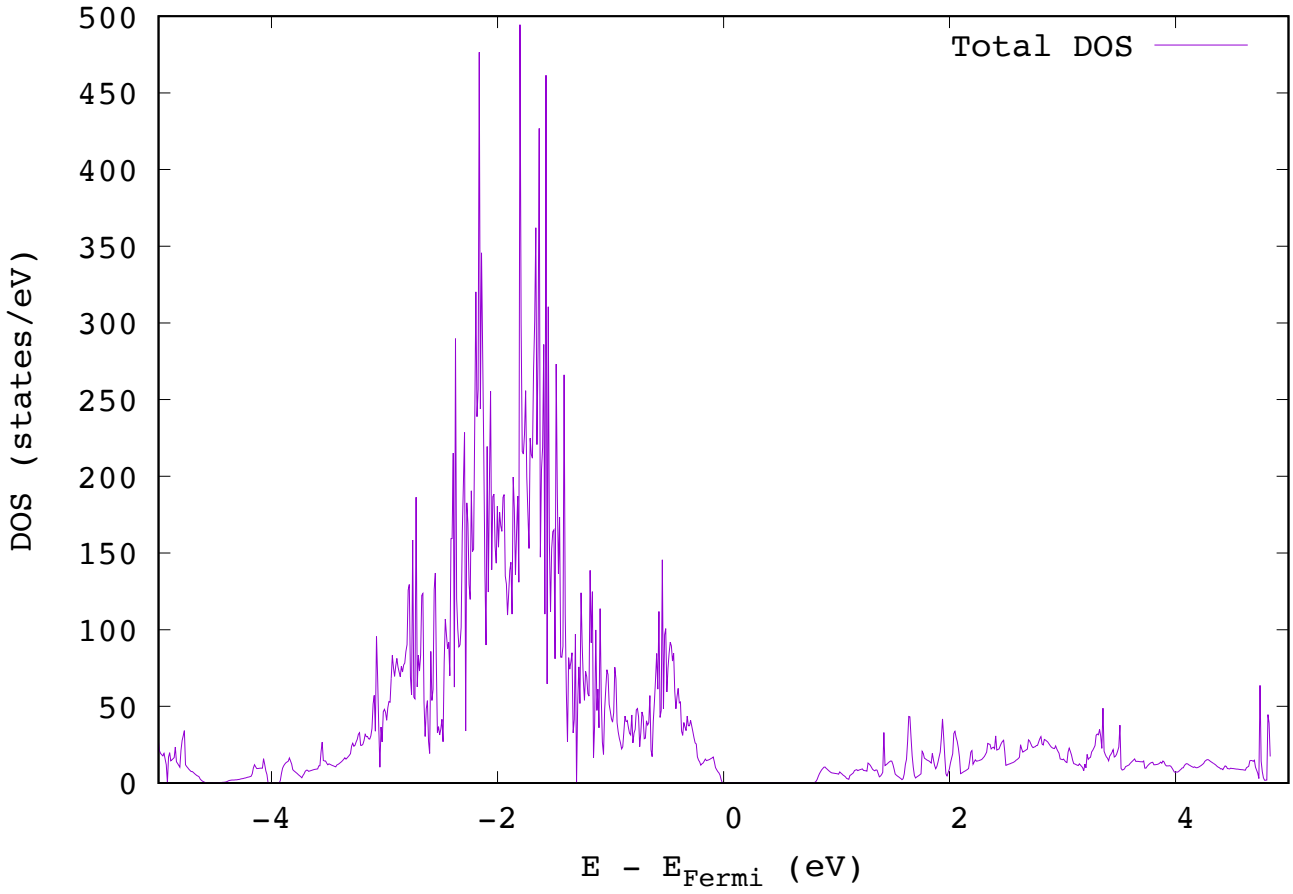
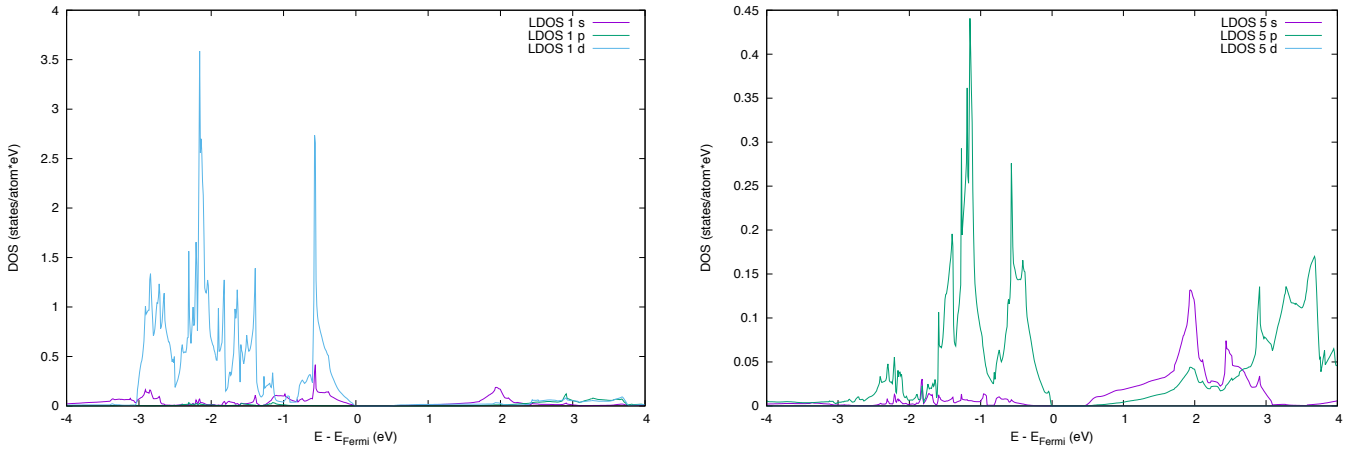

Total DOS
DOS (states/eV)
500
450
400
350
300
250
200
150
100
50
0
-4
-2
0
2
4
E - E_Fermi (eV)

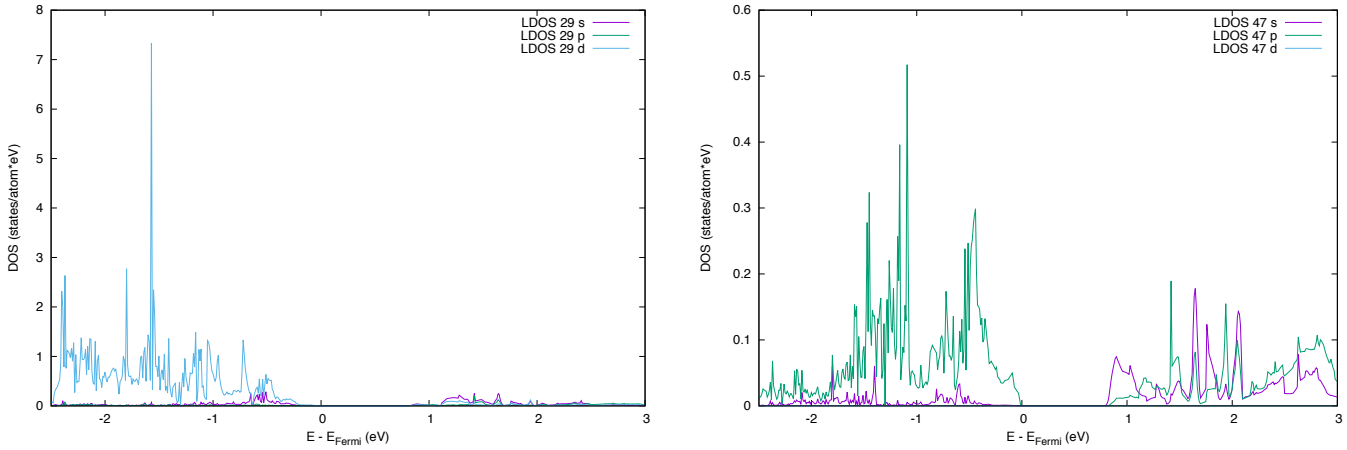
Figure 6.3

6.4.1 LDOS



(a) (b)

Figure 6.4



(a) Cu (b) O

Figure 6.5

7 Discussion

8 Conclusion

References

[1] Vincent E. Lamberti, Lloyd D. Fosdick, Elizabeth R. Jessup, and Carolyn J. C. Schauble. A hands-on introduction to molecular dynamics. *Journal of Chemical Education*, 79(5):601, 2002.

[2] Martin O Steinhauser and Stefan Hiermaier. A review of computational methods in materials science: Examples from shock-wave and polymer physics. *International Journal of Molecular Sciences*, 10(12):5135–5216, 12 2009.

[3] J. Gorecki and J. Gryko. Molecular dynamics simulation of a chemical reaction. *Computer Physics Communications*, 54(2):245 – 249, 1989.

[4] Martin Karplus and Gregory A. Petsko. Molecular dynamics simulations in biology. *Nature*, 347:631 EP –, 10 1990.

Appendix