

FYS4460 -  
First compulsory project

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**1 Abstract**

**2 Model development**

key-words: statefiles, crystal structure, motion(integrator, periodic boundary conditions, forces), MD-units.

**3 Macroscopic observables**

key-words: velocity distributions, tidsutvikling av energi, fluktuasjoner, temperature, pressure, results.

**4 The diffusion constant**

key-word: find it! radial distribution functions.

**5 Thermostats**

key-words: Berendsen, Andersen