

Molecular Statistics, Exam Projects



2015

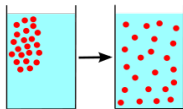
Projects

1. Diffusion Coefficient of the Lennard-Jones Fluid (**JCK**)
2. Genetic Algorithm (**JCK**)
3. Ising Spin-Lattice (**LAB**)
4. Chemical Shifts Study (**LAB**)

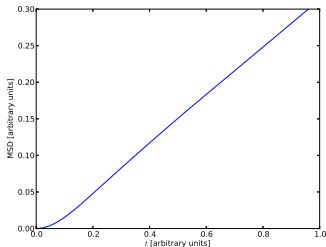


Project 1: Diffusion Coefficient

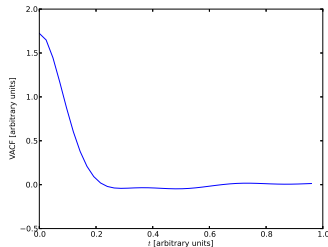
Self-diffusion in Lennard-Jones Fluid.



Mean-Square Displacement



Velocity Auto-Correlation Function



$$D = \lim_{t \rightarrow \infty} \frac{\text{MSD}(t)}{4t} = \frac{1}{2} \int_0^{\infty} \text{VACF}(t) dt$$



Project 1: Diffusion Coefficient

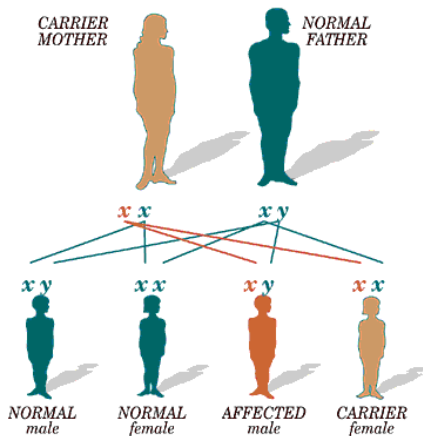
Project description:

- Simulate diffusion under different simulation conditions (pressure, temperature, etc.) using MD in Python.
- Calculate MSD and VACF.
- Calculate diffusion coefficients.



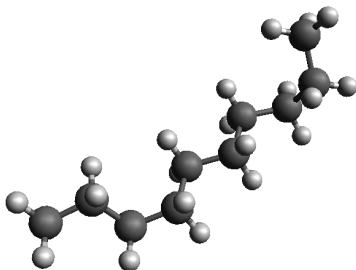
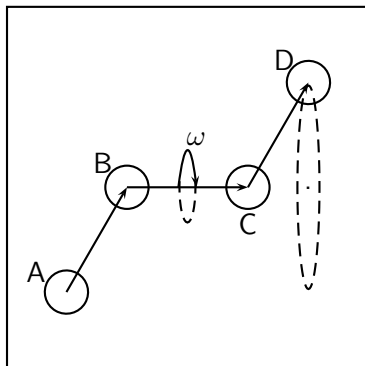
Project 2: Genetic Algorithm

Genetic Algorithm



Project 2: Genetic Algorithm

Energy as a function of dihedral angles



Project 2: Genetic Algorithm



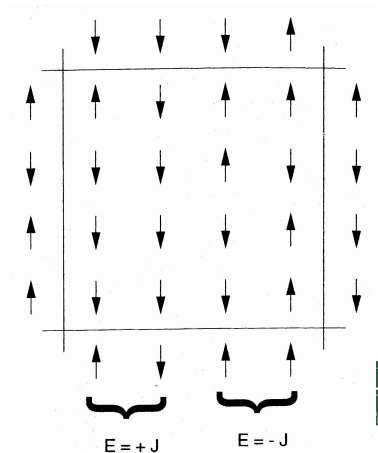
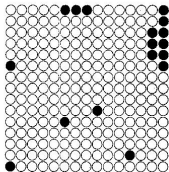
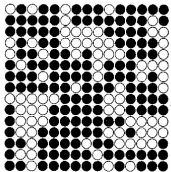
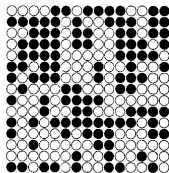
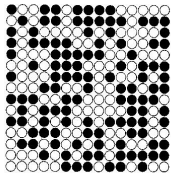
Project description:

- Implement the genetic algorithm in Python.
- Use a force field to calculate molecular energies.
- Use the genetic algorithm to energy minimize alkane molecular structures.



Project 3: 2D Ising Model

Representation of 2D magnetic solid



Project 3: 2D Ising Model

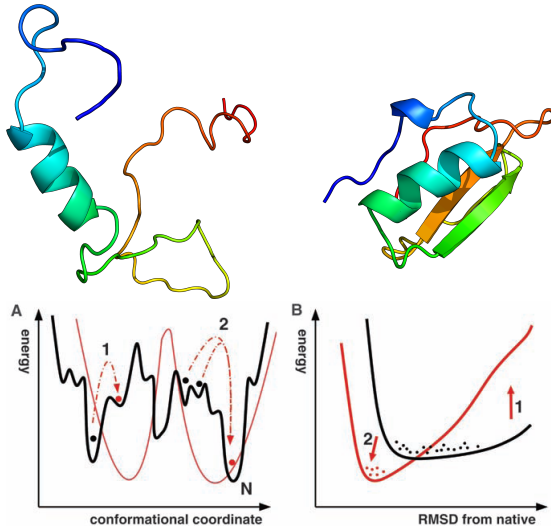
Project description:

- Simulate the 2D Ising spin lattice.
- Implement the Monte Carlo Metropolis-Hastings algorithm.
- Calculate properties such as heat capacity, magnetization, and magnetic susceptibility.



Project 4: Chemical Shifts Study

Using chemical shifts to determine protein structures.



Project 4: Chemical Shifts Study

Project description:

- Parse and analyze simulation data.
- Look for correlations between observables and suggest improvements to model.
- Fit statistical models.



Project description

General:

- Programming is done in small groups
- The reports are individual.
- The language is Danish or English.

Supervisor:

- Jimmy is supervisor for **Genetic Algorithm** and **Diffusion**.
- Lars is supervisor for **Ising-model**.

if stuck:

1. Collaborate with other groups.
2. Write an email and make an appointment to meet with the supervisor.

