Lecture 6 – questions & survey

Answer with yes/maybe/no:

1. What defines the nature of a chemical bond at a fundamental level.
2. Name and define three pair potentials.
3. Explain generally how you identify the parameters of a LJ potential.
4. Explain the specific numerical/algorithm steps in force calculation in a pair potential MD model.
5. Explain the concept of a cutoff radius in a pair potential.
6. Names several brittle materials (examples).
7. Describe the basic mechanisms in brittle fracture.
8. Describe how you can develop a model (interatomic potential and setup) for brittle fracture.

On a scale from 1-7 please rate:

8. Were the goals of today's lecture clear?
9. Was today's lecture clear?
10. Did you feel that today's lecture contributed to your understanding of the topic?
11. What could have been improved in order to make this lecture more useful?
12. Is the level of teaching appropriate? What should we change?
13. Please give us overall feedback regarding IM/S so far how interesting are lectures, overall impression, suggestions for changes, etc.).

Pair potential formulation

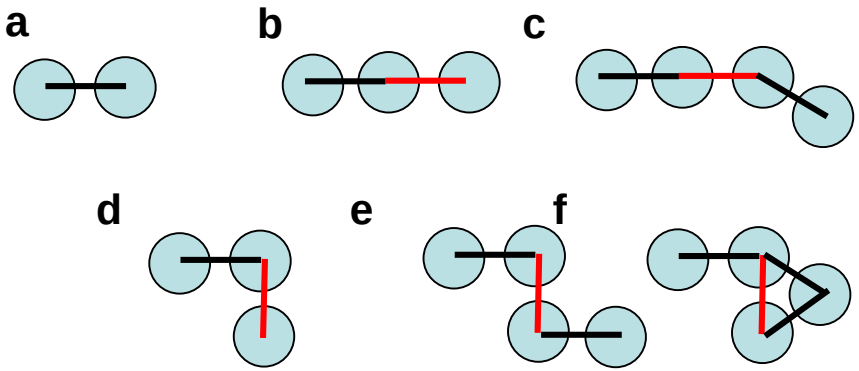
1. List **all parameters** and their respective dimension for the following pair potentials:

   Lennard-Jones
   Morse
   Harmonic

2. Explain the **physical meaning** of each parameter in the **harmonic potential.**

3. Explain the **physical meaning** of each parameter in the **Morse potential.** To solve this problem sketch the Morse potential for different parameter choices and observe changes in the potential shape.

4. Calculate the **potential energy** for the structures shown below (lines between atoms indicate equal distance at r_0), for a Morse pair potential, with cutoff $r_{cut} = 1.1\ r_0$



Morse potential

$$\phi(r_{ij}) = D\exp\left(-2\alpha(r_{ij}-r_0)\right) - 2D\exp\left(-\alpha(r_{ij}-r_0)\right)$$

Lennard-Jones (LJ) potential

$$\phi(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$

Harmonic potential

$$\phi(r_{ij}) = a_0 + \frac{1}{2}k(r_{ij}-r_0)^2$$