

Lecture 8 – questions & survey

Answer with yes/maybe/no:

1. How many amino acids do we have in proteins?
 2. What is the difference between secondary and tertiary structure of a protein?
 3. How many components do we have in CHARMM to describe covalent bonds?
 4. What do we use SMD for?
 5. What is the energy of a single H-bond?
 6. Explain the Bell model
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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

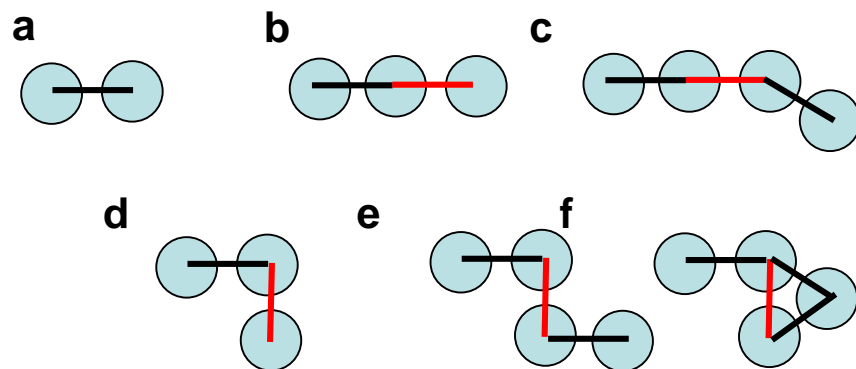
1. List **all parameters** and their respective dimension for the following pair potentials:

- 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 $r_{\text{cut}} = 1.1 r_0$



Morse potential

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

Lennard-Jones (LJ) potential

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

Harmonic potential

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