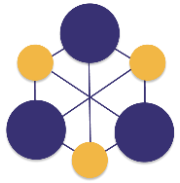

The Lennard Jones Equation

Chem 280

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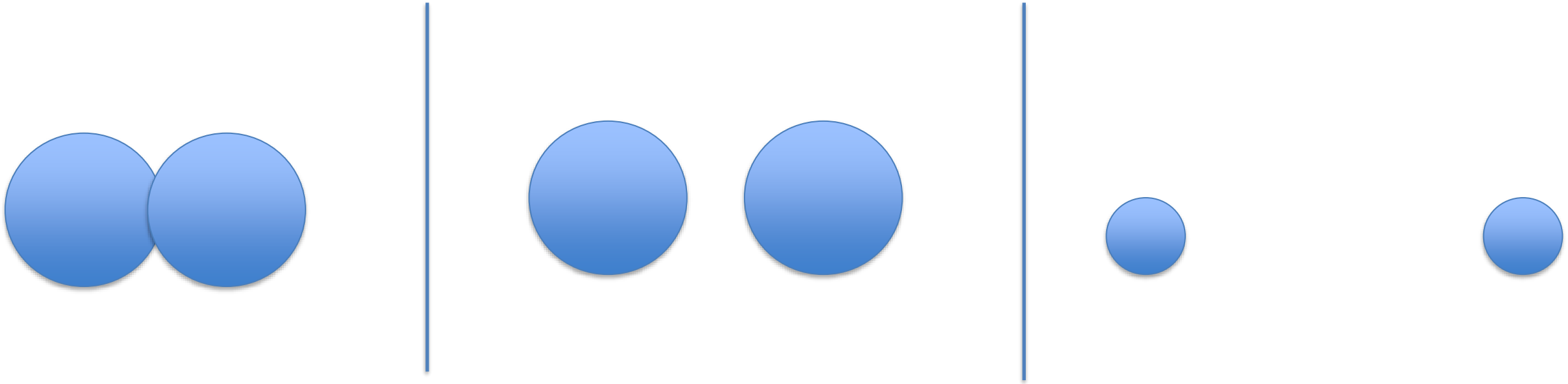
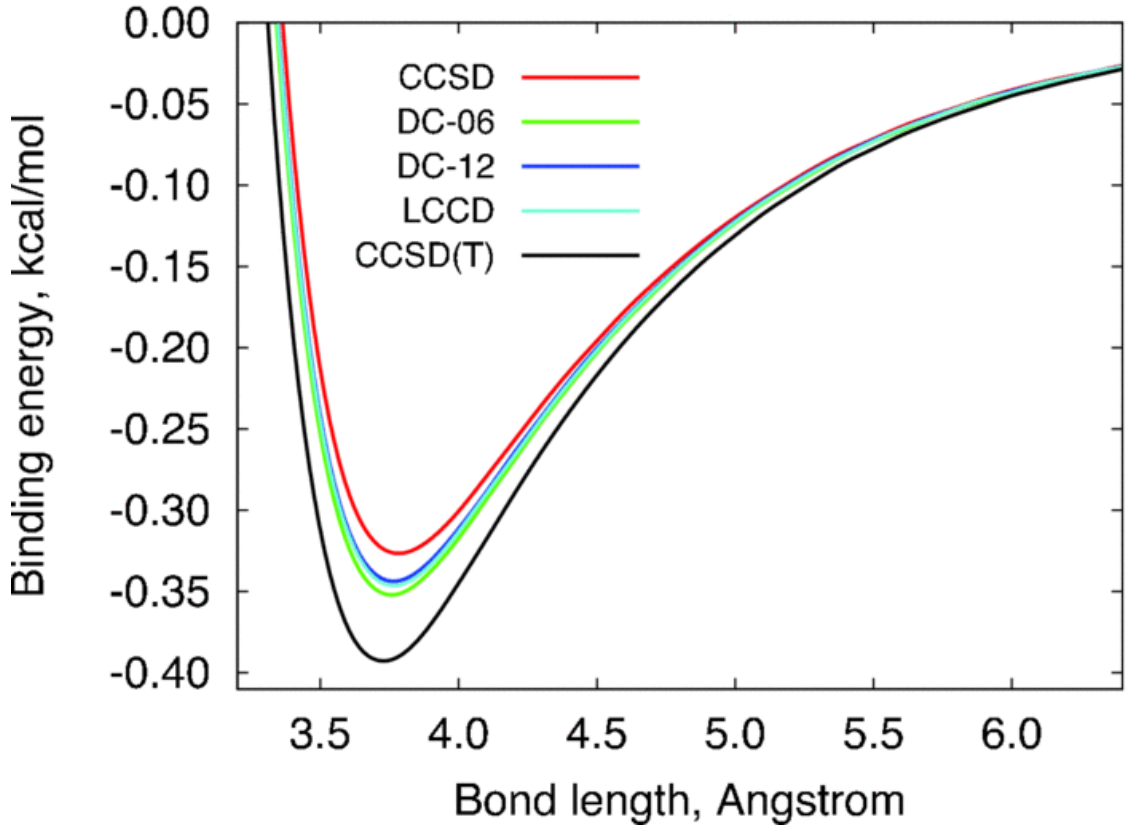
Imagine two interacting atoms



Which one is the highest energy? Why?
Which one is the lowest energy? Why?

“Potential Energy Surface”



Binding potential energy of the argon dimer as a function of Ar–Ar distance computed using different quantum chemistry methods.

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Density cumulant functional theory: The DC-12 method, an improved description of the one-particle density matrix - Scientific Figure on ResearchGate. Available from: https://www.researchgate.net/figure/Binding-potential-energy-of-the-argon-dimer-as-a-function-of-Ar-Ar-distance-computed_fig3_234140936 [accessed 1 Aug, 2023]

The Lennard Jones Equation

- The Lennard Jones equation is an **empirical equation** that models the potential energy interaction of two nonbonded atoms.
  - Empirical equation means that it is based on experimental observations (so not on QM calculations, like the previous slide, though the graphs look similar)
  - First formulated in 1924 by John Lennard-Jones – most common functional form used for modeling nonbonded interactions.

$$Q(r^N) = U(r) = 4\varepsilon[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}]$$

The Lennard Jones Equation