1 Reading assignment 6. Force field

Find the reference philips2005 in the course materials. Read pages 1781 to 1783 and answer the following:

1. Which of Newton's laws is depicted in equation 1?

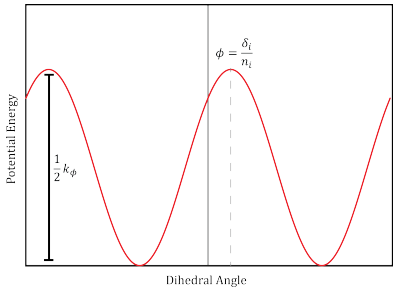
   Newton's second law: $F = ma$

2. What equation corresponds to Hooke's law?

   Equations 3 and 4.

3. What do the curves defined by equations 5 and 6 look like?

   Equation 5 looks like a cosine. Equation 6 shows that at higher distance between two atoms, the van der Waals potential tends to zero (no energy), but when they touch, forms an inverse parable (attraction), and reaching zero it goes to infinite (repulsion).



(a) Equation 5

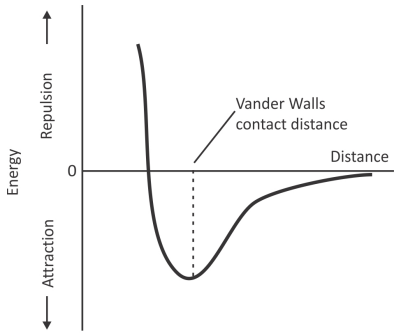


Fig. : Energy graph of Vander Wall's interaction.

(b) Equation 6

4. What is an "improper" dihedral?

   In four atoms covalently bonded in different way, where there is a central atom with three connected atoms, while doing simulations the central atom tends to go to one side of the plane created between the other three atoms (creating angles, like a tent or a pyramid), but no the the opposite one.

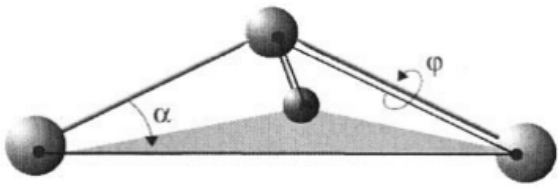


Figure 2. Internal coordinates for bonded interactions: r governs bond stretching; θ represents the bond angle term; ϕ gives the dihedral angle; the small out-of-plane angle α is governed by the so-called "improper" dihedral angle φ.