LECTURE #19 :
3.11 MECHANICS OF MATERIALS F03

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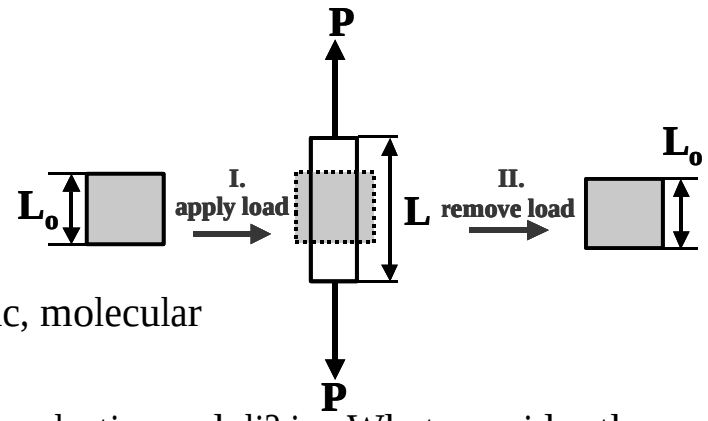
- **REVIEW : INTRODUCTION TO THE MOLECULAR ORIGINS OF MECHANICAL PROPERTIES**
- **QUANTITATIVE TREATMENT OF INTERATOMIC BONDING : THE LENNARD-JONES POTENTIAL**

SUMMARY : LAST LECTURE

I. Basic Definitions :



- elasticity & elastic moduli
  - Young's modulus
  - shear modulus
  - bulk modulus
- *length scales* : macroscopic, microscopic, molecular

II. Questions :

⇒1. What is the molecular origin of the elastic moduli? i.e. What provides the internal resistance to external mechanical forces and deformations and allows materials to hold their shape?

⇒ 2. Why do different materials have vastly different elastic moduli?

⇒ 3. Why do some materials have one elastic moduli (E=constant, isotropic) while other s have different ones in different directions (anisotropic, $E=E(\theta)$?

III. Answers :

⇒ 1. The **TYPE** of internal "cohesive" forces/ bonding/ molecular structure holding the material together.

⇒ 2. How these forces are **ARRANGED** within the material (e.g the placement, packing, and location).

⇒ 3. The **NUMBER** of bonds/unit volume or unit area

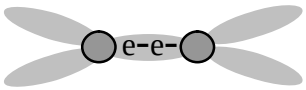
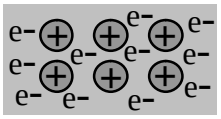
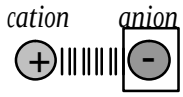
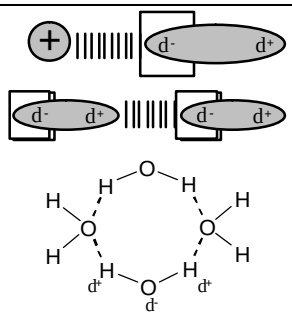
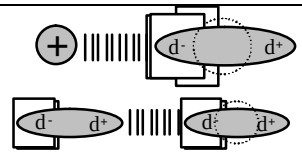
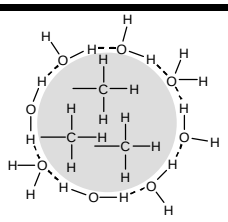
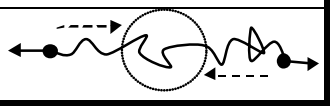
IV. Thermodynamic Contributions to Elastic Moduli :

Molecular Origin	(1) Energetic or Enthalpic	(2) Entropic
macroscopic result	linear elasticity⇒Hooke's Law $\sigma=E\varepsilon$	nonlinear elasticity⇒Rubber Elasticity
strain range	small strains	large strains
material	metals, ceramics, crystalline materials	polymers, rubber networks

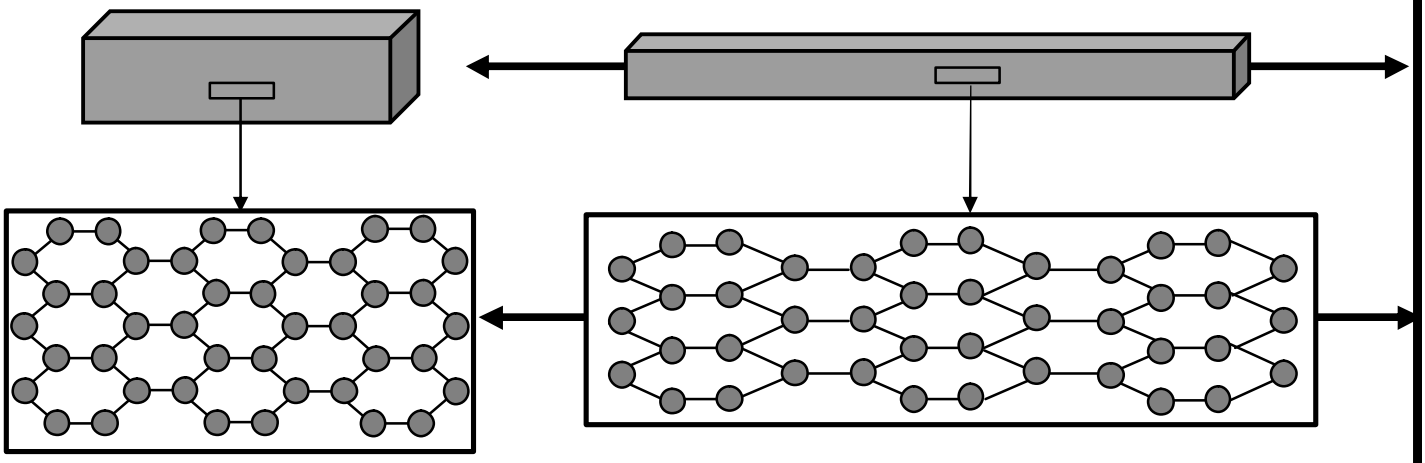
V. Enthalpic Origin of Elastic Moduli:

- distortion of chemical and physical bonds : types
- lattice strain in crystalline materials

Summary of Types of Bonding

Type of Interaction	Classification	Characteristics	Schematic
Covalent :	**Primary or Chemical Bonds :** • usually characterized as individually "strong" • outer orbital e- cooperatively shared between two or more atoms so that discrete nature of atoms is lost • quantum mechanical in origin	• e- are localized • directional (i.e. oriented at well-defined angles to each other)	
Metallic :		• only metals atoms are involved • e- are completely delocalized and mobile throughout entire material • non-directional	
Ionic : • ion-ion		• coulombic in origin, occurs between oppositely charged species • electron transfer from one atom to another	
Polar Interactions : • charge-dipole • dipole-dipole • hydrogen bonding	**Secondary or Physical Interactions :** • usually characterized as individually "weak" • no e- sharing, more subtle attraction between (+) and (-) charges, discrete nature of atoms preserved • typically exhibits : • lack of specificity • lack of directionality • lack of stoichiometry	• force between an ion and a dipole or two dipoles where the (+) charge attracts the (-) charge (purely electrostatic) • *H-bonding* : a special type of dipole-dipole interaction that results from the bonding between a H atom which is partially (+) charged and a highly electronegative atom such as O, F, N, Cl, (directional)	
Polarization Interactions : • charge-nonpolar (induced or instantaneous dipole) • dipole-nonpolar (induced dipole)		• an ion or dipole in the vicinity of a nonpolar atom or molecule causes instantaneous polarization and electrostatic attraction	
Dispersion or London Interactions : (*also called charge-fluctuation, electrodynamic, induced-dipole-induced dipole forces) • nonpolar-nonpolar		• the (+) nucleus of a nonpolar atom attracts the (-) charged electrons of another nonpolar atom resulting in instantaneous, induced, dipoles and fluctuating electron clouds • quantum mechanical in origin	
Hydrophobic :	**Special Interactions :** • not really true "bonds" • non-directional	• attraction between nonpolar molecules in aqueous solution caused by their inability to form H-bonds with HOH so as to minimize the disruption of H-bonds in HOH • entropy-driven	
Entropic Elasticity :		• attractive, recoiling force produced via extensional deformation macromolecules	

Atomistic Basis for Elasticity: One Example : Crystalline Materials



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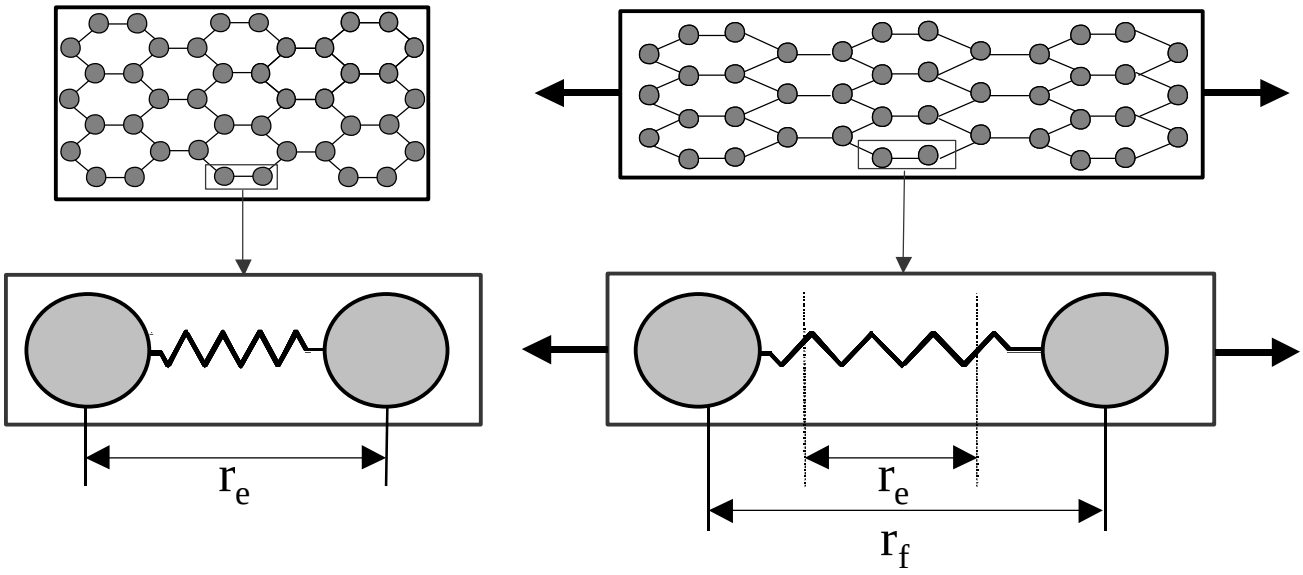
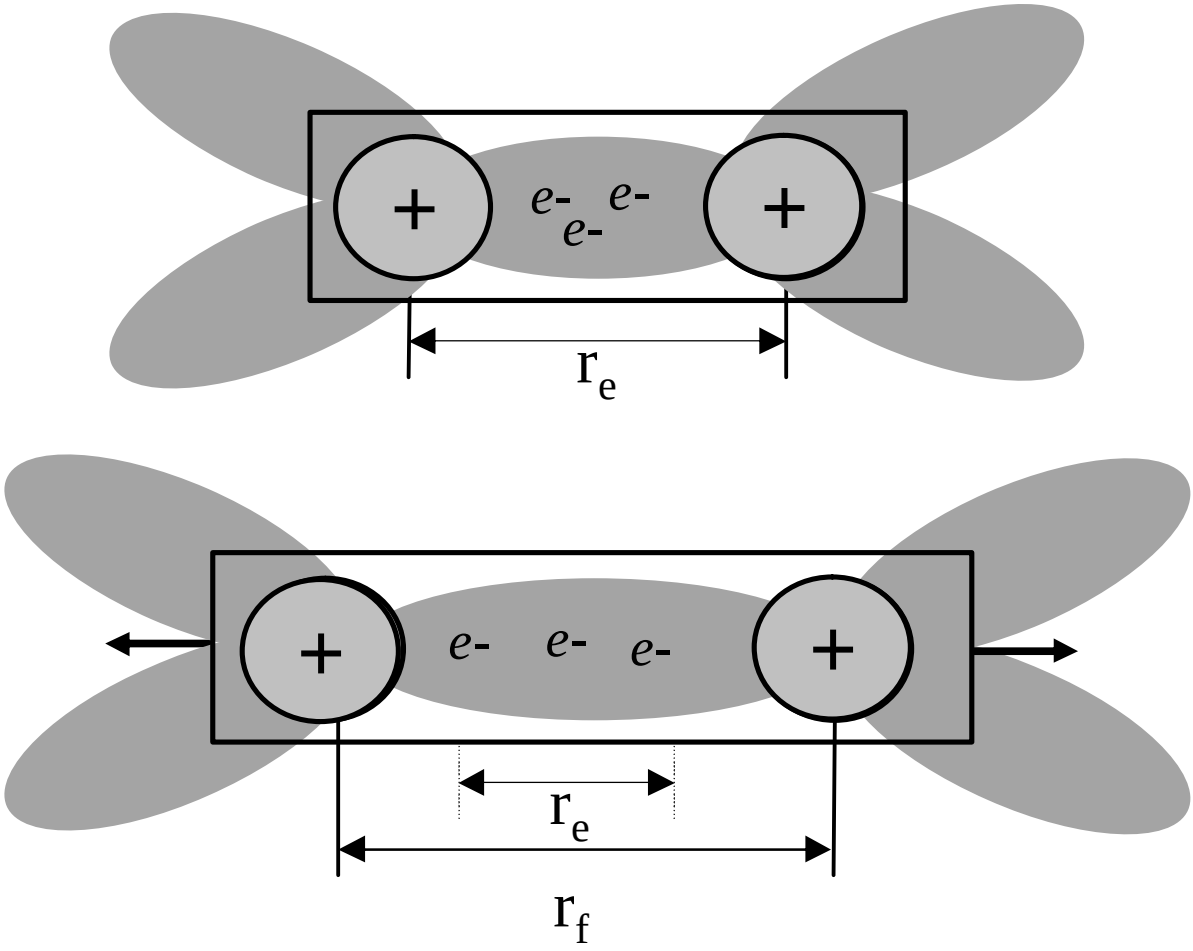


Atomistic Basis for Elasticity:

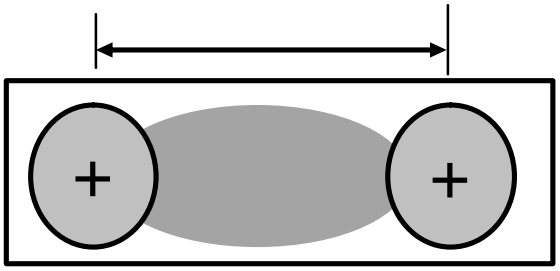
covalent bond : outer orbitals cooperatively shared



lattice strain disturbs electronic configuration

Consider an Individual Bond

interatomic distance, r (nm)

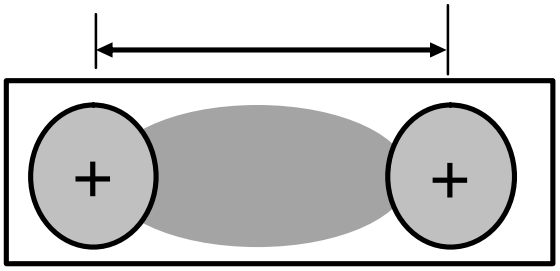


interatomic (bond) energy, *W* (kJ / mol)

interatomic force, F (nN)

Interaction Parameters

interatomic distance, r (nm)



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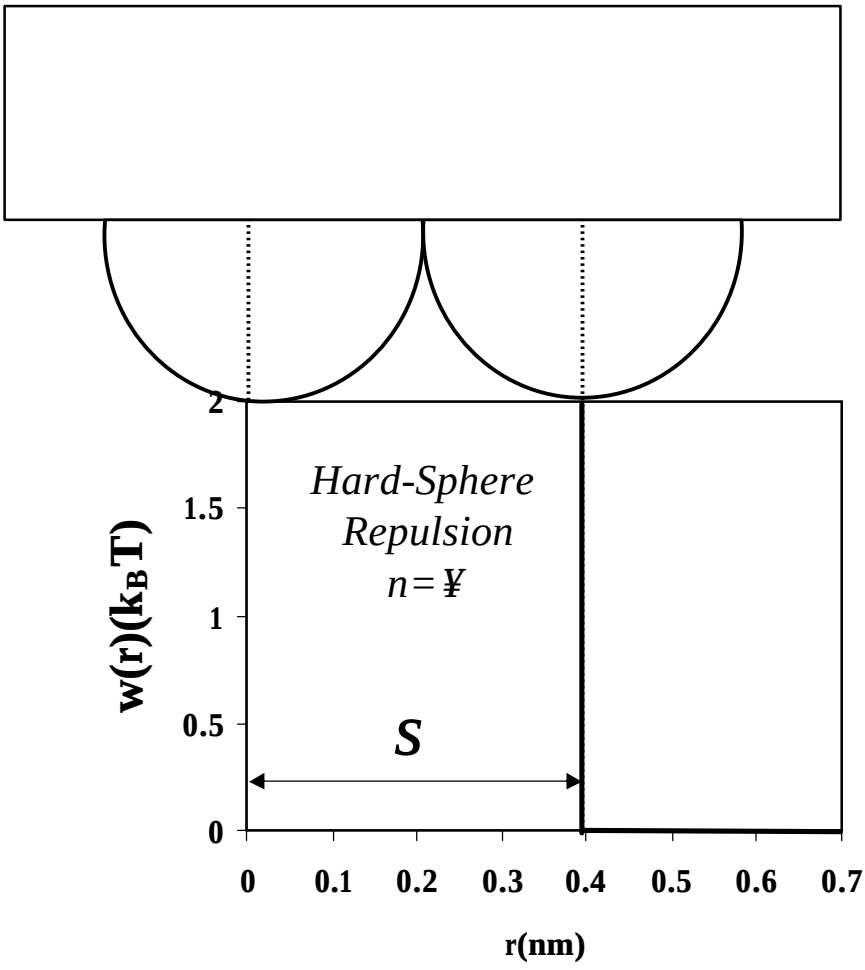
Molecular Origin of Repulsive Component



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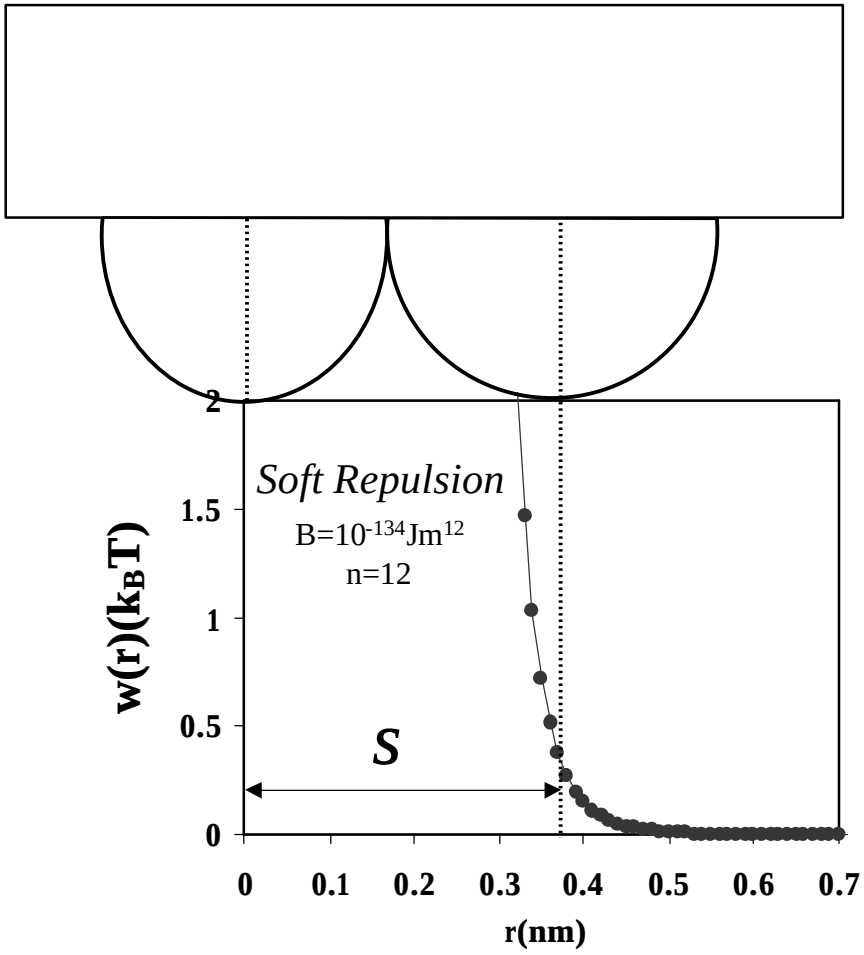
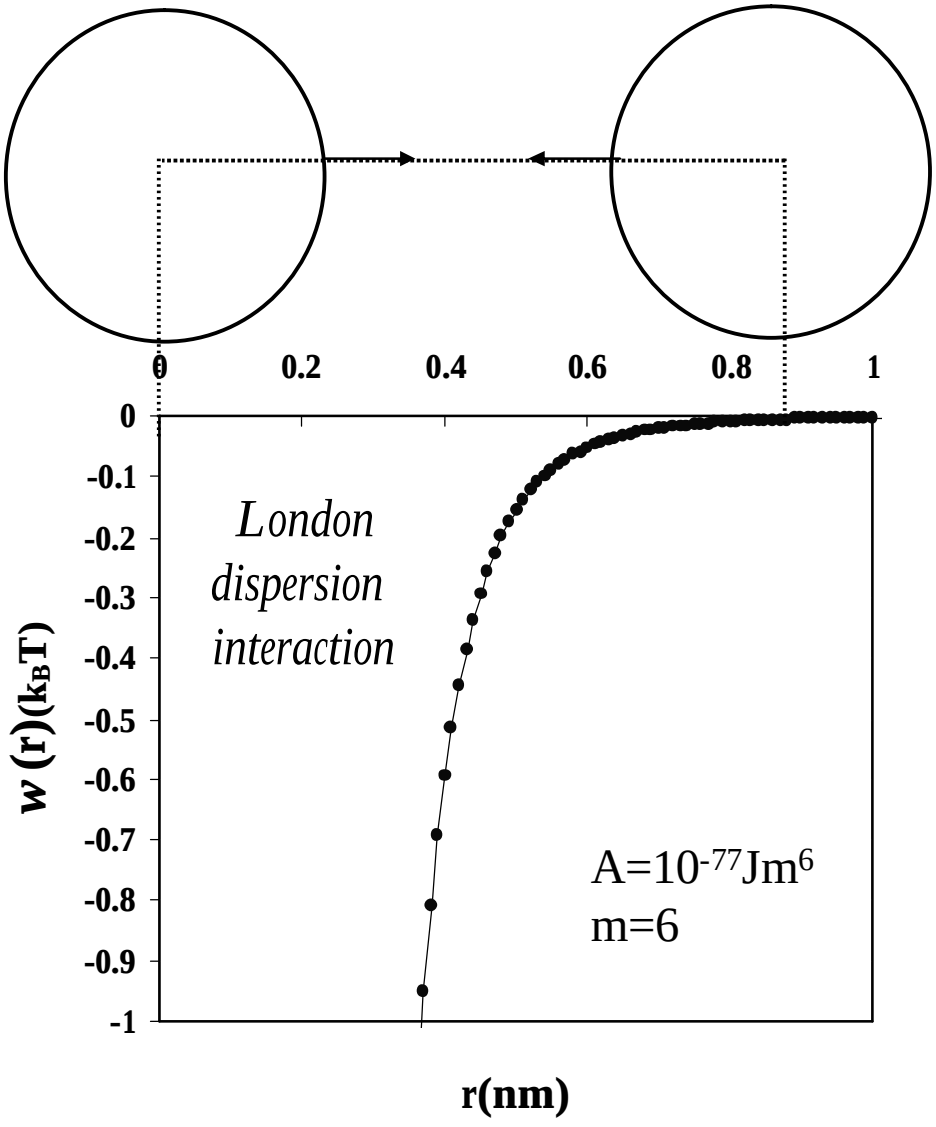
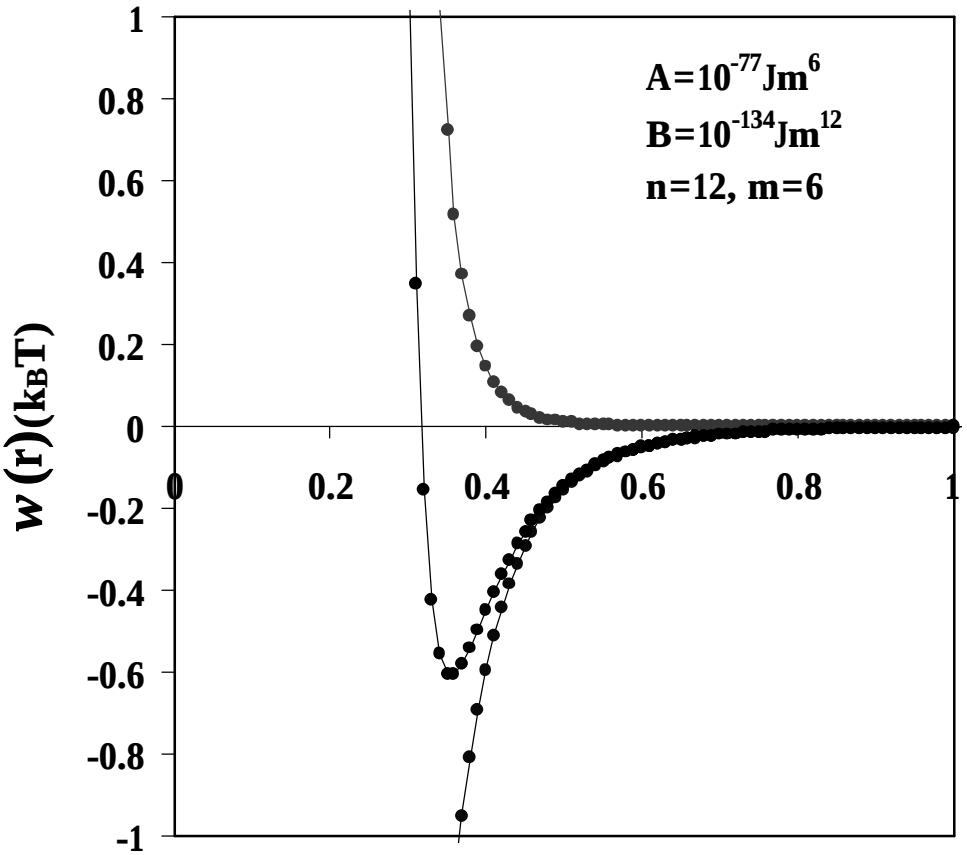


Molecular Origin of Attractive Component



Complete Interaction Potential : "The Lennard-Jones Potential"



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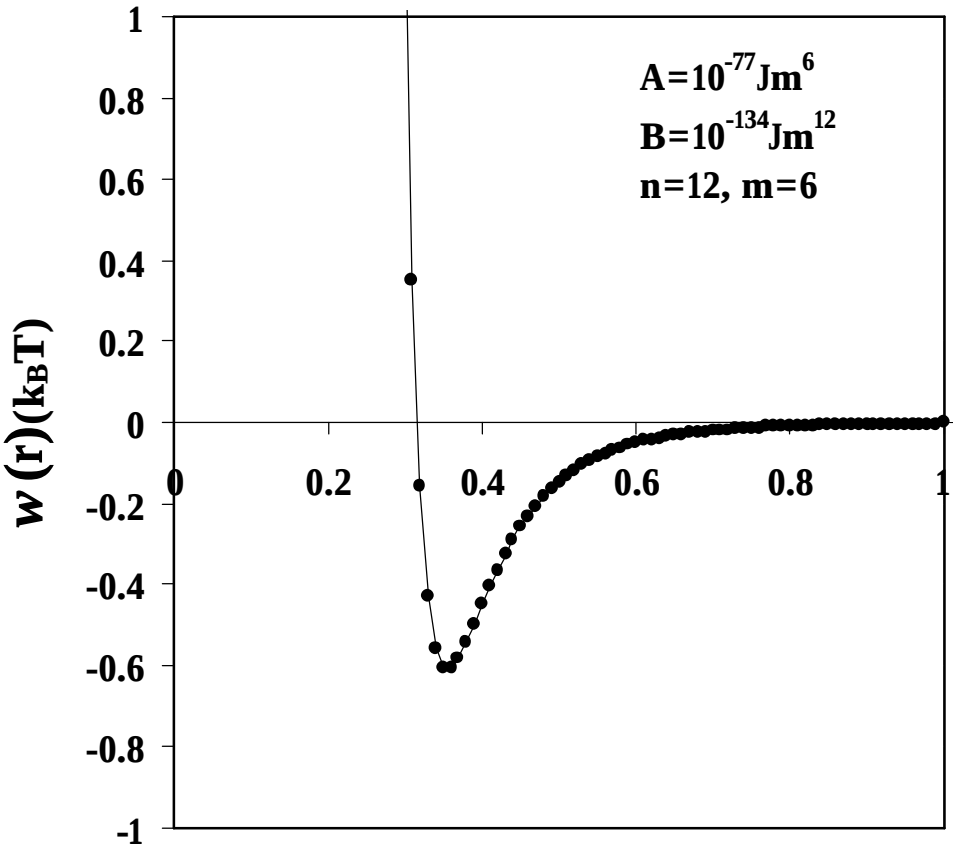
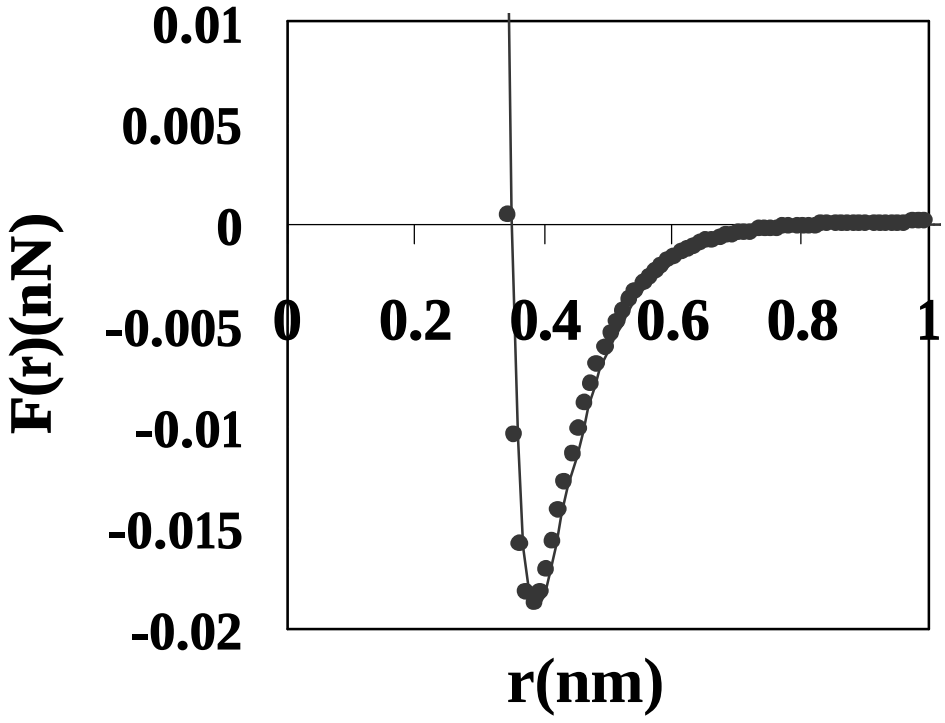


Interaction Force :



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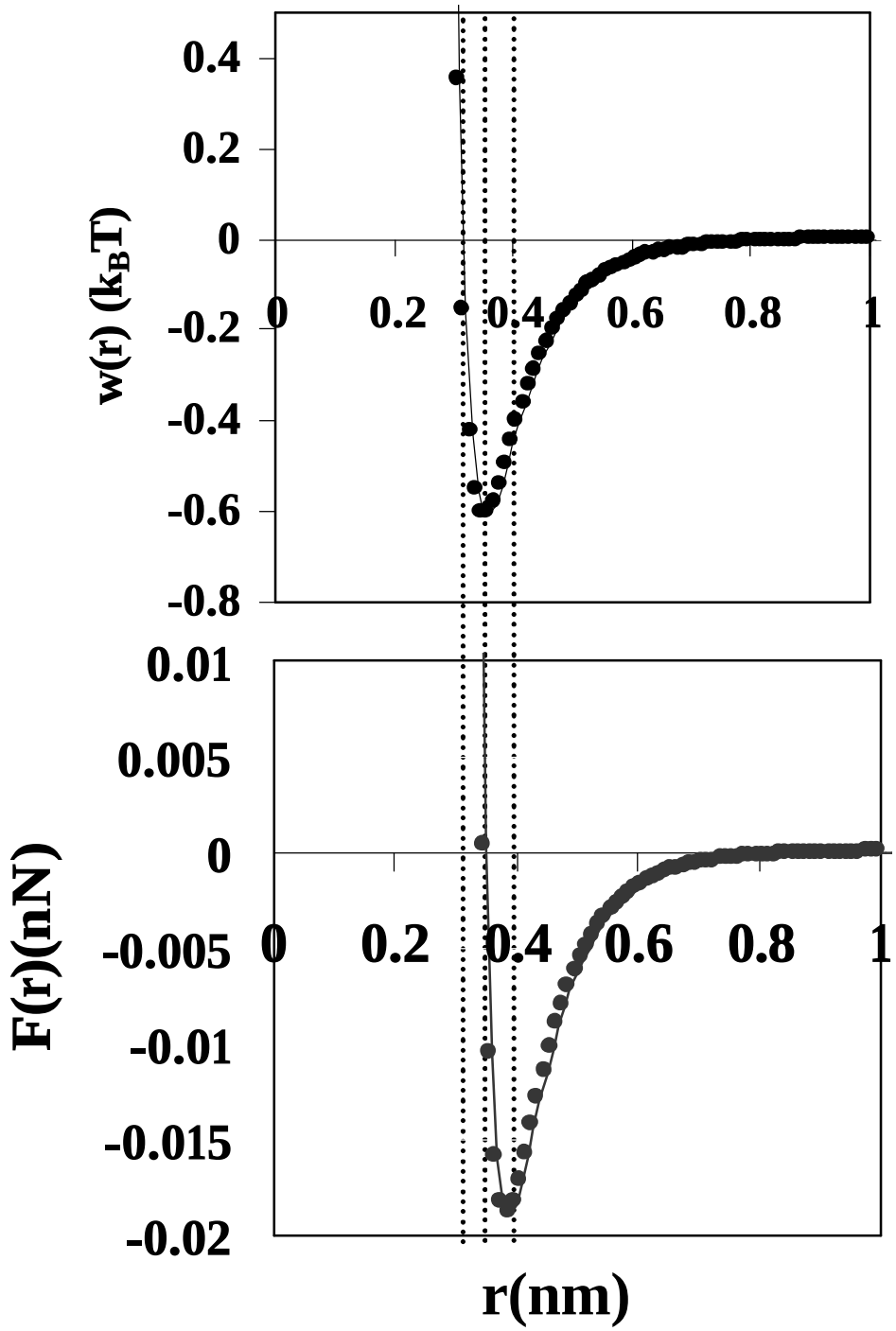

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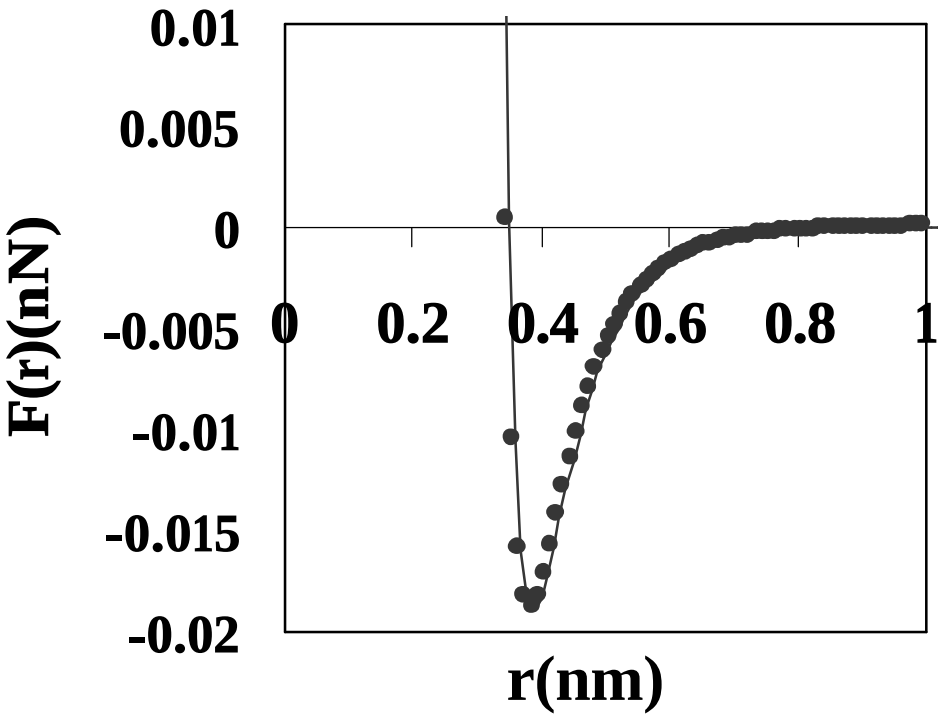

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