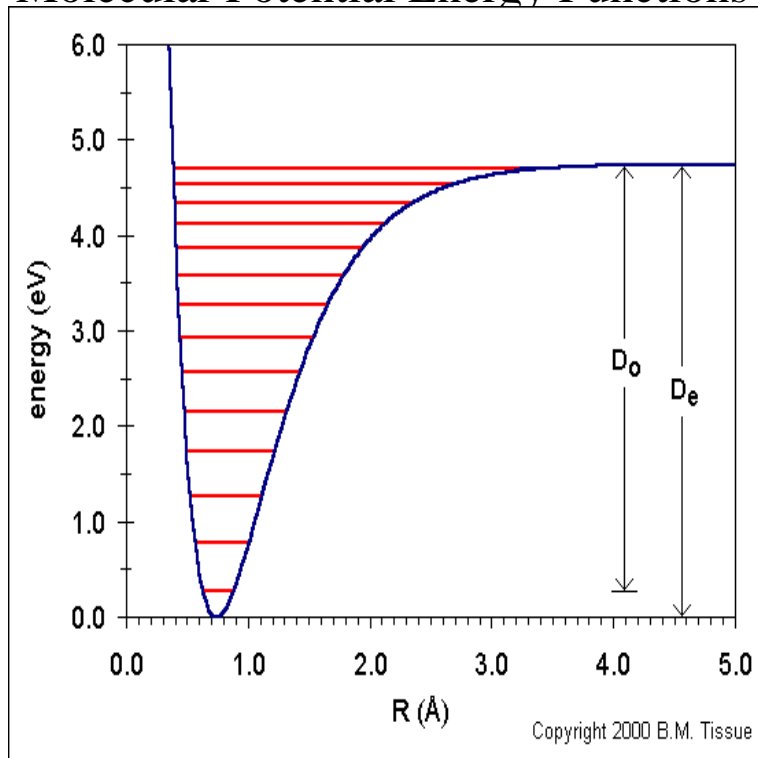


Molecular Potential Energy Functions



The states expected to be populated at thermal equilibrium are the low-energy regions of this (potential) energy function, and forces on individual atoms are related to the gradient of this function, which is why such functions are also commonly referred to as force fields. Potential energy functions. We called the function a "potential" energy function as it does not contain contributions made to the total energy made by the motions of the atoms involved. It is possible to calculate these using molecular dynamics methods. Evaluating the force is the most computationally demanding part of molecular dynamics. The force is the negative gradient of a scalar potential energy function. Theoretical studies of biological molecules permit the study of the relationships between structure, function and dynamics at the atomic level. Since many of the. THE development of an intermolecular potential energy function for simple molecules based solely on an investigation of properties arising from two-body. A series of papers describing advances made in recent years in obtaining explicit functions for the potential energy surfaces of small polyatomic molecules. Molecular Potential Energy Functions. To cite this article: M S Child Phys. Bull. 36 View the article online for updates and enhancements.

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