A Study on Mechanics and Nanosystems

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A technological revolution has begun and it is in our power to organize and manipulate matter starting from an atomic level as well as to design tools, machinery, and energy conversion devices in nano scale toward the development of nanotechnology.

The systems of interest to nano science and nanotechnology are the isolated individual nanostructures and their assemblies. Nano systems are made of limited number of atoms or molecules. Their sizes are larger than individual molecules and smaller than microsystems. One of the characteristic features of nano systems is their high surface-to- volume ratio. Their electronic and magnetic properties are often distinguished by quantum mechanical behavior, whereas their mechanical properties can be formulated within the framework of classical statistical mechanics of small systems, now known as nonex- tensive statistical mechanics, as it is discussed in this chapter. Nano systems can contain all forms of condensed matter, be it soft or hard, organic or anorganic. A deep understanding of the interactions between individual atoms and molecules composing the nanosystems and their statistical mechanical modeling is essential for nano-technology.

This study is concerned with one of the most important subjects of computational nano technology; eg. statistical mechanical modeling and its application to molecular systems to predict the properties of nano scale structures. The modification and implementation of statistical mechanics for nano scale systems would lead to possibilities to study the evolution of physical, chemical, and biophysical systems on significantly reduced length,

time, and energy scales. The statistical mechanical modeling and its application to nanosystems is achieved through mathematical modeling and computer-based molecular simulations employing concepts from statistical mechanics of large systems as well as quantum mechanical many-body theories. If performed correctly, it can provide insight into the formation, evolution, and properties of nano structures and their relation with macroscopic behavior of matter.

The *computer-based simulation methods*, being developed for nano systems, consist of a computational procedure performed on a limited number of atoms, molecules, confined to a limited, but small space. The most important input to such computation is the energy function for interaction between the entities composing the nano system. Accurately administered computer simulations can help in three different ways: First, they can be used to compare and evaluate various molecular- based theoretical models. For this purpose, we can use the same potential function in the simulation as well as in the theoretical calculation. Second, for nano systems, computer simulations can help evaluate and direct an experimental procedure that otherwise may not be. Third, an use of computer simulation is its potential to replace an experiment, provided accurate intermolecular potentials are available to be used in their development. Methods used for simulation of several properties of nano scale systems differ in their level of accuracy and in the computer time necessary to perform such calculations.