Insights Into Mesoscopic, Micro-heterogeneous and Fluctuating Systems by Molecular Modeling and Simulations

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Molecular simulations are becoming common tools in physics and engineering for investigating several scientific problems. One may wonder about the success of these techniques, used only few years ago to describe the behaviour of model systems, too simple to even qualitatively describe complex systems or to quantitatively describe experimental systems. The truth is that simulations have greatly contributed to improve our knowledge of complex systems where many competing effects may hide the relevant physics leading the behaviour of the system; furthermore, they are used nowadays as standard tools in academia and industry to predict the behaviour of systems for which a limited set of experimental data is available and/or for extreme conditions, difficult to reach experimentally. The key of the success of molecular simulations for several practical problems lies not only in the increased computer power, which overcomes some of the limitations encountered few years ago, but also in the development of new intelligent algorithms and in the development of more accurate force fields for several purposes. We will first briefly introduce some of the most recent advances in this field followed by some specific applications such as the simultaneous prediction of phase and interface properties by direct molecular dynamic simulations and the behavior of nanoparticles at liquid-liquid interfaces. The influence of temperature and molecular parameters on the interfacial properties of these systems will be discussed in detail.