Theoretical Study of the Effect of Phospholipid Bilayer in the Electronic Properties of Molecules with Biophysical Interest.

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also proven impressive. Since energetic frustration is sufficiently small, native structure-based models, which correspond to perfectly unfrustrated energy landscapes, have shown to be a powerful approach to explore larger proteins and protein complexes, not only folding but also function associated to large conformational motions. Therefore a discussion of how global motions control the mechanistic processes in the ribosome and molecular motors will be presented. For example, this conceptual framework is allowing us to envisage the dynamics of molecular motors from the structural perspective and it provides the means to make several quantitative predictions that can be tested by experiments. For different kinesin motors (kinesin-1 and ncd), a prototype of the biological machines in the cell, structure-based molecular simulations of these explicit kinesins and microtubule structures were used to glean a number of salient features that supplement the current experimental findings.

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Solvent effects are of essential importance in many different aspects of physics, chemistry, biology and material sciences. The developments of quantum chemistry methods originally devised for studying isolated molecules have been extended to study the properties of atoms and molecules interacting with the environment. This led to the continuum methods that treat the solvent by means of average macroscopic constants, such as the dielectric constants. Very successful in different applications these continuum methods lack the consideration of the microscopic details and the necessary statistic representation of the thermodynamic molecular system. The natural extension has been to incorporate some molecular mechanics methods to generate solute-solvent structures and couple this with the quantum mechanical methods to obtain the solvent effects in the solute properties. This is the

essence of the so-called QM/MM methods where part of the system is treated by molecular mechanics (MM) whereas the remaining is treated by quantum mechanics (QM). We have been involved in the developments of a sequential procedure (S-QM/MM)[1] where the MM simulations are used to obtain the structures of the solution for subsequent QM calculations. In this presentation we report some developments [2,3] of this methodology and we address to some applications in electronic polarization and spectrum for some organic molecules in different environments, such as homogeneous liquid [4-5] and phospholipid membranes [6].

Keywords: Electronic properties, heterogeneous medium, mixture, bilayer.
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Manipulating Protein Stability: Enthalpy vs Entropy

The thermodynamic stability is among the most important biophysical characteristics of proteins. The stability may dictate many other features of the protein, such as its structural integrity, its fluctuations and thus its