From molecules to proteins: new perspectives of computational chemistry

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ABSTRACT

Detection of simplest organic molecules in the interstellar space (ISM), prebiotic molecules evolution toward more complex species and biomolecules self-assembly and structure-function relations are nowadays studied by broad range of spectroscopic techniques. Majority of molecular structures have been obtained from X-ray crystallography or microwave (MW) spectroscopy. On the other hand, structure and properties can be monitored by different spectroscopic measurements such as infrared (IR), Raman, Resonance Raman, UV-vis absorption or fluorescence or circular dichroism (CD), electron spin resonance (ESR). However, it is seldom straightforward to link the rich experimental data to the desired information on the specific structure and properties of complex molecular systems. Moreover, traditionally, these experimental results have been analysed separately. Quantum chemistry computations yield direct information on all possible properties of molecular systems, some of them very difficult to obtain from experiment. That provides a missing link between different experimental techniques, which could not be integrated and fully explored otherwise.

I will discuss status and perspective of the project aimed at structure and spectroscopy studies for systems of increasing size and complexity, from small prebiotic molecules to larger bio-molecules, complexes and proteins. Step-by-step strategy starts from comparison with highly accurate theoretical models and/or state-of-the art experimental data for smaller systems, gradually moving towards larger and more complex molecular systems featuring dispersion interactions, hydrogen bonding, variable local stereochemistry-conformation, and chirality.

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