Environmental Effects in Computational Spectroscopy: Accuracy and Interpretation

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Spectroscopic techniques are valuable tools for understanding the structure and dynamics of complex systems, such as biomolecules or nanomaterials. Most of the current research is devoted to the development of new experimental techniques for improving the intrinsic resolution of different spectra. However, the subtle interplay of several different effects acting at different length and time scales still makes the interpretation and analysis of such spectra a very difficult task. In this respect, computational spectroscopy is becoming a needful and versatile tool for the assignment and interpretation of experimental spectra. It is in fact possible nowadays to model with relatively high accuracy the physical–chemical properties of complex molecules in different environments, and to link spectroscopic evidence directly to the structural and dynamical properties of optically or magnetically active solvated probes. In this Review, significant steps toward the simulation of entire spectra in condensed phases are presented together with some basic aspects of computational spectroscopy, which highlight how intramolecular and intermolecular degrees of freedom influence several spectroscopic parameters.

Słowa kluczowe

ab initio calculations, computational chemistry, computational spectroscopy, density functional calculations, spectroscopy

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