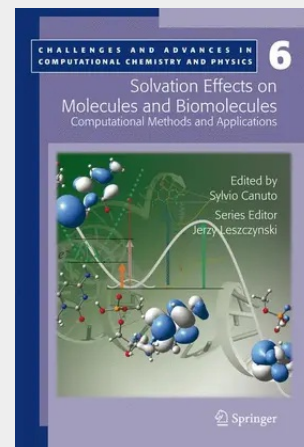


Solvation Effects on Molecules and Biomolecules

Computational Methods and Applications

The incessant development of quantum chemistry since the appearance of the Schrödinger equation has turned this area into a respectable branch of science with unprecedented capabilities. It is now a well-recognized field of research with predictive power that is an important component in physical-chemical laboratories. Very important developments were conducted in the early days by bright theoretical scientists that were ready to absorb the incredible and unpredicted computer revolution which was only just beginning. Isolated medium-size molecular systems can now be accurately studied theoretically by quantum chemical methods. However, it was also long recognized that all biomolecular phenomena necessary to obtain and sustain living systems take place in solution, as well as the vast majority of chemical processes. Indeed solvent and liquid systems are germane in chemistry experiments. In physics, a constant concern is the description of the role played by the environment in modifying the properties of the system as compared to the isolated situation. Hence, the importance of studying atoms, molecules and biomolecules in the solvent environment can hardly be denied. The quantum chemical studies of molecular systems affected by the interaction with a solvent had its own turning point before the end of the 1970s, when some pioneering work was done, including the dielectric properties of the medium in an effective nonlinear Hamiltonian. This naturally led to the development of the so-called continuum models that are important and now popular. Continuum models can be implemented from the simplest to the most sophisticated quantum chemical methods.

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