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Sommario/riassunto

There have been important developments in the last decade: computers are faster and more powerful, code features are enhanced and more efficient, and larger molecules can be studied - not only in vacuum but also in a solvent or in crystal. Researchers are using new techniques to study larger systems and obtain more accurate results. This is impetus for the development of more efficient methods based on the first-principle multi-level simulations appropriate for complex species. Among the cutting-edge methods and studies reviewed in this decennial volume of the series are the Density Function