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Quantum Chemistry: Fundamentals to Applications

Tamás Veszprémi, Miklós Fehér



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`Quantum Chemistry [the branch of Computational Chemistry that applies the laws of Quantum Mechanics to chemical systems] is one of the most dynamic fields of contemporary chemistry, providing a solid foundation for all of chemistry, and serving as the basis for practical, computational methodologies with applications in virtually all branches of chemistry ... The increased sophistication, accuracy and scope of the theory of chemistry are due to a large extent to the spectacular development of quantum chemistry, and in this book the authors have made a remarkable effort to provide a modern account of the field.' From the Foreword by Paul Mezey, University of Saskatchewan.

Quantum Chemistry: Fundamentals to Applications develops quantum chemistry all the way from the fundamentals, found in Part I, through the applications that make up Part II. The applications include:

- molecular structure;
- spectroscopy;
- thermodynamics;
- chemical reactions;
- solvent effects; and
- excited state chemistry.

The importance of this field is underscored by the fact that the 1998 Nobel Prize in Chemistry was awarded for the development of Quantum Chemistry.

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