



Computational Quantum Chemistry: Molecular Structure and Properties In Silico (RSC Theoretical and Computational Chemistry Series)

Joseph J W McDouall

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Computational Quantum Chemistry presents computational electronic structure theory as practised in terms of ab initio waveform methods and density functional approaches. Getting a full grasp of the field can often prove difficult, since essential topics fall outside of the scope of conventional chemistry education. This professional reference book provides a comprehensive introduction to the field.

Postgraduate students and experienced researchers alike will appreciate Joseph McDouall's engaging writing style. The book is divided into five chapters, each providing a major aspect of the field. Electronic structure methods, the computation of molecular properties, methods for analysing the output from computations and the importance of relativistic effects on molecular properties are also discussed. Links to the websites of widely used software packages are provided so that the reader can gain first hand experience of using the techniques described in the book.

Dr McDouall has more than 25 years experience in theoretical chemistry; as a reader at the University of Manchester his research interests include the application of quantum chemical methods to the elucidation of chemical problems and the development and implementation of electronic structure methods that permit the accurate prediction of chemical structures and molecular properties.

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