



Multiconfigurational Quantum Chemistry

Björn O. Roos, Roland Lindh, Per Åke Malmqvist, Valera Veryazov, Per-Olof Widmark

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The first book to aid in the understanding of multiconfigurational quantum chemistry, *Multiconfigurational Quantum Chemistry* demystifies a subject that has historically been considered difficult to learn. Accessible to any reader with a background in quantum mechanics and quantum chemistry, the book contains illustrative examples showing how these methods can be used in various areas of chemistry, such as chemical reactions in ground and excited states, transition metal and other heavy element systems. The authors detail the drawbacks and limitations of DFT and coupled-cluster based methods and offer alternative, wavefunction-based methods more suitable for smaller molecules.

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