

## Handbook of electronic structure theory : methods and applications

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### Kolekcja

Naukowa

### Język

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### Streszczenie

*Handbook of Electronic Structure Theory: Methods and Applications* provides a much-needed learning resource that collects and demonstrates the various key methods involved in electronic structure theory, the feasibility and reliability of electronic structure calculations, and their applications using computational chemistry. With a particular focus on the most modern and recent problems that are typically poorly covered in existing, largely outdated book literature, this handbook is designed with early career researchers in mind. It is written primarily for masters, PhD, and postdoctoral students in theoretical and computational chemistry as well as experimental researchers wishing to apply quantum chemical methods in a critical way.

Elements like summary boxes, worked examples, and downloadable datasets make this a holistic guide to the topic for learners from different backgrounds who require a deeper understanding of electronic structure theory. Sections focus on critical core theories, the most important recent developments, and future directions, including key topics such as the electronic excited states and the harnessing of machine learning. Finally, the book collects a range of key case study examples of applications, such as in biomolecules, in spectroscopy, and for use in catalysis, amongst others.

### Adres publiczny

<https://www.sciencedirect.com/book/edited-volume/9780443265969/handbook-of-electronic-structure-theory>