Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Comprehensive Computational Chemistry. Vol. 2, The Analysis of chemical bonding and the interpretation of wave functions

Autorzy

Sławomir Berski

Redaktorzy

Manuel Yáñez

Russell J. Boyd

Rok wydania

2024

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Streszczenie

Comprehensive Computational Chemistry stands as an authoritative publication, comprising over 150 chapters that encompass the entire spectrum of the field. It delves into the foundational principles of theoretical methods, the development of algorithms and software packages, and their extensive applications in various domains, including atmospheric chemistry, biochemistry, materials science, and medicinal chemistry.

Edited by a team of world-renowned scientists, this four-volume set covers everything from the theoretical foundations of quantum chemistry to the intricacies of modeling chemical reactions, exploring excited electronic states, and delving into the dynamics of molecular systems. It also sheds light on the critical role of computational chemistry in understanding and designing highly specific and efficient catalysts for various applications.

Whether you are entering the field, an accomplished scientist, or an ambitious undergraduate student, "Comprehensive Computational Chemistry" is an invaluable resource for navigating the ever-evolving landscape of computational chemistry.

Computational chemistry is a rapidly evolving discipline with growing relevance in various scientific domains. This groundbreaking reference resource is poised to shape the trajectory of the field and push its boundaries into uncharted territories.

Słowa kluczowe

computational chemistry

Adres publiczny

https://www.sciencedirect.com/referencework/9780128232569/compreher computational-chemistry

Plik został wygenerowany dnia 2026-11-09 19:36:28

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/gnG-m82.