1. Record Nr. UNINA9910143176403321

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Titolo	Reviews in computational chemistry . Volume 17 / / Donald B. Boyd, Kenny B. Lipkowitz, Thomas R. Cundari
Pubbl/distr/stampa	New York, NY : , : John Wiley & Sons, Inc., , [2001] ©2001
ISBN	1-280-36631-1 9786610366316 0-470-35124-1 0-471-45881-3 0-471-22441-3
Edizione	[1st ed.]
Descrizione fisica	1 online resource (431 p.)
Collana	Reviews in computational chmistry ; ; 17
Disciplina	542.85
Soggetti	Chemistry - Data processing Chemistry - Research Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di contenuto	Reviews in Computational Chemistry Volume 17; Preface; Contents; Contributors; Contributors to Previous Volumes*; 1. Small Molecule Docking and Scoring; Introduction; Algorithms for Molecular Docking; The Docking Problem; Placing Fragments and Rigid Molecules; Flexible Ligand Docking; Handling Protein Flexibility; Docking of Combinatorial Libraries; Scoring; Shape and Chemical Complementary Scores; Force Field Scoring; Empirical Scoring Functions; Knowledge-Based Scoring Functions; Comparing Scoring Functions in Docking Experiments: Consensus Scoring From Molecular Docking to Virtual ScreeningProtein Data Preparation; Ligand Database Preparation; Docking Calculation; Postprocessing; Applications; Docking as a Virtual Screening Tool; Docking as a Ligand Design Tool; Concluding Remarks; Acknowledgments; References; 2. Protein-Protein Docking; Introduction; Why This Topic?; Protein-Protein Binding Data; Challenges for Computational Docking Studies; Computational Approaches to the Docking Problem; Docking =

Sampling + Scoring; Rigid-Body Docking; Flexible Docking; Example; Estimating the Extent of Conformational Change upon Binding Rigid-Body DockingFlexible Docking with Side-Chain Flexibility; Flexible Docking with Full Flexibility; Future Directions; Conclusions; References; 3. Spin-Orbit Coupling in Molecules; What It Is All About; The Fourth Electronic Degree of Freedom; The Stern-Gerlach Experiment; Zeeman Spectroscopy; Spin Is a Quantum Effect; Angular Momenta; Orbital Angular Momentum; General Angular Momenta; Spin Angular Momentum; Spin-Orbit Hamiltonians; Full One- and Two-Electron Spin-Orbit Operators; Valence-Only Spin-Orbit Hamiltonians; Effective One-Electron Spin-Orbit Hamiltonians; Symmetry Transformation Properties of the Wave FunctionTransformation Properties of the Hamiltonian; Matrix Elements; Examples; Summary; Computational Aspects; General Considerations; Evaluation of Spin-Orbit Integrals; Perturbational Approaches to Spin-Orbit Coupling; Variational Procedures; Comparison of Fine-Structure Splittings with Experiment; First-Order Spin-Orbit Splitting; Second-Order Spin-Orbit Splitting; Spin-Forbidden Transitions; Radiative Transitions; Nonradiative Transitions; Summary and Outlook; Acknowledgments; References; 4. Cellular Automata Models of Aqueous Solution Systems IntroductionCellular Automata; Historical Background; The General Structure; Cell Movement; Movement (Transition) Rules; Collection of Data; Aqueous Solution Systems; Water as a System; The Molecular Model; Significance of the Rules; Studies of Water and Solution Phenomena; A Cellular Automata Model of Water; The Hydrophobic Effect; Solute Dissolution; Aqueous Diffusion; Immiscible Liquids and Partitioning; Micelle Formation; Membrane Permeability; Acid Dissociation; Percolation; Solution Kinetic Models; First-Order Kinetics; Kinetic and Thermodynamic Reaction Control; Excited-State Kinetics Second-Order Kinetics

Sommario/riassunto

Computational chemistry is increasingly used in most areas of molecular science including organic, inorganic, medicinal, biological, physical, and analytical chemistry. Researchers in these fields who do molecular modelling need to understand and stay current with recent developments. This volume, like those prior to it, features chapters by experts in various fields of computational chemistry. Two chapters focus on molecular docking, one of which relates to drug discovery and cheminformatics and the other to proteomics. In addition, this volume contains tutorials on spin-orbit coupling and ce

2. Record Nr. UNINA9910808679003321

Autore	Campbell D (David)
Titolo	German infantryman versus Soviet rifleman : Barbarossa 1941 / / David Campbell
Pubbl/distr/stampa	Oxford, England ; ; New York, New York : , : Osprey Publishing, , 2014 ©2014
ISBN	1-4728-0326-4 1-4728-0325-6
Descrizione fisica	1 online resource (202 p.)
Collana	Combat
Disciplina	358.43
Soggetti	World War, 1939-1945 - Campaigns - Soviet Union World War, 1939-1945 - Campaigns - Eastern Front Soviet Union History German occupation, 1941-1944
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Cover; Title; Contents; Introduction; The Opposing Sides; Zhlobin; Smolensk; Vas'Kovo-Voroshilovo; Analysis; Aftermath; Unit Organizations; Bibliography; Imprint
Sommario/riassunto	The Axis invasion of the Soviet Union on 22 June 1941 pitted Nazi Germany and her allies against Stalin's forces in a mighty struggle for survival. Fighting alongside the spearhead Panzer divisions were Germany's highly skilled and veteran motorized infantrymen - including the German Army's premier unit, Infanterie-Regiment (mot.) Grossdeutschland. Opposing these German mobile forces, the Soviets deployed the often ill-trained and poorly equipped men of the rifle regiments, who fought tenaciously and with the threat of savage reprisals from their own side. In this book three bruising clashe