1. Record Nr. UNINA9910863155103321

Titolo	QM/MM Studies of Light-responsive Biological Systems / / edited by Tadeusz Andruniów, Massimo Olivucci
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2021
ISBN	3-030-57721-X
Edizione	[1st ed. 2021.]
Descrizione fisica	1 online resource (XVI, 336 p. 97 illus., 89 illus. in color.)
Collana	Challenges and Advances in Computational Chemistry and Physics, , 2542-4483 ; ; 31
Disciplina	571.455
Soggetti	Chemistry, Physical and theoretical Bioinformatics Spectrum analysis Proteins Theoretical Chemistry Physical Chemistry Computational and Systems Biology Spectroscopy Protein Biochemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes index.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	On the Automatic Construction of QM/MM Models for Biological Photoreceptors: Rhodopsins as Model Systems -- Photo-Active Biological Molecular Materials: From Photoinduced Dynamics to Transient Electronic Spectroscopies -- Polarizable Embedding as a Tool to Address Light-Responsive Biological Systems -- Computational Studies of Photochemistry in Phytochrome Proteins -- QM/MM Study of Bioluminescent Systems -- QM/MM Approaches Shed Light on GFP Puzzles -- DNA Photodamage and Repair: Computational Photobiology in Action.
Sommario/riassunto	This book, a consecutive contribution to the series Challenges and Advances in Computational Chemistry and Physics, focuses on understanding the photoinduced processes in biological systems. Understanding and fine control of light fate in molecules is vital for the

progress of society and environmental safety. Light induced changes of various physico-chemical and spectroscopic properties in nucleic acids and proteins is the basis of fundamental biological events such as vision, DNA photodamage or photosensing. The investigation of these processes is challenging to both theoretical and experimental studies. This volume encompasses the quantum mechanics/molecular mechanics theory in several subfields, including: advanced computational methods for nucleic acids and proteins systems; dynamics, spectroscopic and physico-chemical properties of biological photoreceptors; DNA photodamage. This book is of interest to readers in both fundamental and application-oriented research by overviewing recent achievements in computational modeling of excited states in nucleic acids and proteins.