

Computational Photochemistry (Theoretical and Computational Chemistry)



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Computational Photochemistry, Volume 16 provides an overview of general strategies currently used to investigate photochemical processes. Whilst contributing to establishing a branch of computational chemistry that deals with the properties and reactivity of photoexcited molecules, the book also provides insight into the conceptual and methodological research lines in computational photochemistry. Packed with examples of applications of modelling of basic photochemical reactions and the computer-aided development of novel materials in the field of photodegradation (paints), photoprotection (sunscreens), color regulation (photochromic devices) and fluorescent probes, this book is particularly useful to anyone interested in the effect of light on molecules and materials.

* Provides an overview of computational photochemistry, dealing with principles and applications

* Demonstrates techniques that can be used in the computer-aided design of novel photo responsive materials

* Written by experts in computational photochemistry

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