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Autore	Sousa Sergio F
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Sommario/riassunto	Over recent decades, the increase in computational resources, coupled with the popularity of competitive quantum mechanics alternatives (particularly DFT), has promoted the widespread penetration of quantum mechanics calculations into a variety of fields targeting the reactivity of molecules. This book presents a selection of original research papers and review articles illustrating diverse applications of quantum mechanics in the study of problems involving molecules and their reactivity.