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with Large Double Excitation Character

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Sommario/riassunto

Molecular modeling encompasses applied theoretical approaches and computational techniques to model structures and properties of molecular compounds and materials in order to predict and / or interpret their properties. The modeling covered in this book ranges from methods for small chemical to large biological molecules and materials. With its comprehensive coverage of important research fields in molecular and materials science, this is a must-have for all organic, inorganic and biochemists as well as materials scientists interested in applied theoretical and computational chemistry. The 28
