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Sommario/riassunto

This comprehensive book, edited by Shubin Liu, delves into the exploration of chemical concepts through theoretical and computational chemistry. It covers a broad range of topics including molecular orbital theory, valence bond theory, density functional theory, and energy decomposition analysis. The book aims to provide insights into chemical bonding, partial charges, aromaticity, and various other fundamental chemical concepts. The chapters are contributed by numerous experts, offering both static and dynamic properties of chemical entities. This resource is invaluable for researchers, academics, and advanced students in the field of chemistry who are interested in understanding the theoretical underpinnings and computational approaches that define chemical principles and empirical laws.