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Nota di contenuto	1. Physical properties of methane -- 2. Methane hydroxylation by transition-metal oxide ions -- 3. Enzymatic methane hydroxylation by methane monooxyganese -- 4. Methane and benzene oxidation by metal-exchanged zeolites -- 5. Methane activation on metal-oxide surfaces -- 6. Methane activation on alloy surface: Informatics approach -- 7. Synergy of theory and experiment.
Sommario/riassunto	This book focuses on theoretical and computational studies by the editor’s group on the direct hydroxylation of methane, which is one of the most challenging subjects in catalyst chemistry. These studies of more than 20 years include gas-phase reactions by transition-metal oxide ions, enzymatic reactions by two types of methane monooxygenase (soluble and particulate MMO), catalytic reactions by metal-exchanged zeolites, and methane C–H activation by metal oxide surfaces. Catalyst chemistry has been mostly empirical and based on enormous experimental efforts. The subject of the title has been tackled using the orbital interaction and computations based on extended Hückel, DFT, and band structure calculations. The strength of the theoretical studies is in the synergy between theory and experiment. Therefore, the group has close contacts with experimentalists in physical chemistry, catalyst chemistry, bioinorganic chemistry, inorganic chemistry, and surface chemistry. This resulting book will be useful for the theoretical analysis and design of catalysts. .