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Acknowledgments; References; 3 Mechanistic Understanding of Catalytic CO<sub>2</sub> Activation from First Principles Theory; 3.1 Background; 3.2 CO<sub>2</sub> activation and hydrogenation on transition metal surface; 3.2.1 Methanol from CO<sub>2</sub> Hydrogenation on Cu Surfaces; 3.2.2 Methanol from CO<sub>2</sub> Hydrogenation on Modified Cu Surfaces 3.2.3 CO<sub>2</sub> Hydrogenation on Ni(1 1 0) and Ni(1 1 1)3.3 CO<sub>2</sub> activation and hydrogenation on oxide supports; 3.4 CO<sub>2</sub> activation and hydrogenation on oxide supported metal catalysts; 3.5 Concluding Remarks; Acknowledgment; References; 4 Catalytic Activation and Conversion of Carbon Dioxide into Fuels/Value-Added Chemicals Through C-C Bond Formation; 4.1 Introduction; 4.2 Chemical activation of carbon dioxide; 4.2.1 Coordination Chemistry of CO<sub>2</sub> and Metals; 4.2.1.1 Molecular Geometry and Spectroscopic Properties of CO<sub>2</sub>; 4.2.1.2 Interaction of CO<sub>2</sub> with Metals 4.2.2 Synthesis and Characterization of Stable Complexes of CO<sub>2</sub> with Metals 4.2.2.1 General Characterization Methods; 4.2.2.2 Synthesis of Stable CO<sub>2</sub>-Metal Complexes; 4.2.2.3 Stable Complexes of CO<sub>2</sub> Coordinated to Metals; 4.2.2.3.1 Coordination via a C≡O<sub>2</sub>B<sub>8</sub>O double bond; 4.2.2.3.2 Coordination via carbon only; 4.2.2.3.3 Coordination via oxygen only; 4.2.2.3.4 CO<sub>2</sub> as Bridging Ligand; 4.2.3 Reactivity of Complexes of CO<sub>2</sub> with Metals; 4.2.3.1 C-O Bond Cleavage and Oxygen Transfer; 4.2.3.2 Reactions with Electrophiles; 4.2.3.3 Reactions with Nucleophiles 4.2.4 Activation of CO<sub>2</sub> Using N-Heterocyclic Carbenes and FLPs

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#### Sommario/riassunto

New and Future Developments in Catalysis is a package of books that compile the latest ideas concerning alternate and renewable energy sources and the role that catalysis plays in converting new renewable feedstock into biofuels and biochemicals. Both homogeneous and heterogeneous catalysts and catalytic processes will be discussed in a unified and comprehensive approach. There will be extensive cross-referencing within all volumes. This volume presents a complete picture of all carbon dioxide (CO<sub>2</sub>) sources, outlines the environmental concerns regarding CO<sub>2</sub>, and

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