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Catalysis, in the industrial production of chemicals, fuels, and materials, accounts for more than half of gross material production worldwide. Heterogeneous catalysis enables fast and selective chemical transformations, resulting in superior product yield and facilitating catalyst separation and recovery. The synthesis of novel catalysts has emerged as a hot topic for process and product development with numerous research publications and patents. Hence, development of efficient catalysts and their applications is important for sustainable energy production and use, green chemicals production and use, and economic growth. This Special Issue discusses recent developments related to catalysis for the production of sustainable fuels and chemicals and traverses many new frontiers of catalysis including synthesis, characterization, catalytic performances, reaction kinetics and modelling, as well as applications of catalysts for the production of biofuels, synthesis gas, and other green products. This covers the current state-of-the-art catalysis research applied to bioenergy. organic transformation, carbon-carbon and carbon-heteroatoms, reforming, hydrogenation, hydrodesulfurization, hydrodenitrogenation, hydrodemetalization, Fischer-Tropsch synthesis, to name a few. This book highlights new avenues in catalysis including catalyst preparation methods, analytical tools for catalyst characterization, and technoeconomic assessment to enhance a chemical or biological transformation process using catalysts for a betterment of industry,