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Nota di contenuto	Introduction -- Experimental and Theoretical Methods -- Design of Pd-Ni Bimetallic Catalyst -- Effect of Oxide Supports on Pd–Ni Bimetallic Catalysts -- Replacing Precious Metals with Carbide Catalysts -- Liquid Phase Hydrogenation of Acetylene -- Conclusion.
Sommario/riassunto	This thesis offers novel methods for catalyst and process design for the selective hydrogenation of acetylene and 1,3-butadiene. The author predicts the properties of supported Pd–Ni bimetallic catalysts using density functional theory (DFT) calculations and temperature-programmed desorption (TPD). The excellent correlation between model surfaces and supported catalysts demonstrates the feasibility of designing effective bimetallic catalysts for selective hydrogenation reactions. The author also proposes a method for designing non-precious metal catalysts to replace precious metals. She modifies the process of selective hydrogenation of acetylene by coupling the selective adsorption to the selective hydrogenation in the liquid phase,

as a result of which the ethylene selectivity is greatly improved and heat transfer is greatly enhanced. Lastly, by analyzing the mechanism of liquid-phase hydrogenation, the author proposes a multi-stage slurry bed reactor for industrial applications.