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Ph.D. DISSERTATION DEFENSE

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Degree: Doctor of Philosophy
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Title: Molecular Fundamentals of Metal Nanoparticles for Catalytic Selective Hydrogenation and Oxidation of Hydrocarbons

Chairperson: Dr. Simon Podkolzin, Department of Chemical Engineering and Materials Science

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ABSTRACT

Catalytic conversion of hydrocarbons plays a critical role in the production of fuels, chemicals, and materials, contributing significantly to the development of cleaner and more sustainable chemical processes. Among these, selective oxidation and hydrogenation reactions are of particular importance, enabling the transformation of simple feedstocks into valuable intermediates while minimizing energy input and undesired byproducts. The performance of such reactions is largely governed by the physicochemical properties of the catalysts employed. In recent years, metal nanoparticles have emerged as promising catalysts due to their high surface area, tunable surface structures, and ability to form unique active sites when supported on appropriate materials. Understanding the molecular fundamentals that control the activity, selectivity, and stability of these metal nanoparticles remain essential for advancing catalyst design and industrial application.

This dissertation investigates the molecular-level structure and reactivity of metal nanoparticles—primarily gold and palladium—toward catalytic selective oxidation and hydrogenation of hydrocarbons. Using a combination of in situ spectroscopic techniques, electron microscopy, and density functional theory (DFT) calculations, the work reveals the essential roles of particle size, surface structure, and support interactions in controlling catalytic behavior. These studies provide fundamental insights into how nanoscale structure, metal-support interactions, and surface chemistry govern the activity and selectivity of metal catalysts in hydrocarbon transformations. This work contributes to the rational design of next-generation catalysts for energy-efficient and environmentally benign chemical processes.