Research Campaign: An Integrated Multi-Capability Approach for Analysis of Catalytic Systems

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Introduction. In this campaign we will link dynamic measurements with computational capabilities at molecular interfaces to address important questions related to catalysis that stretch across the DOE's scientific and engineering complex. In order to develop and maximize beneficial catalytic outcomes (increased selectivity, enhanced turn-over rates, reduction of hazardous by-products, greater efficiency leading to decreased energy consumption, etc.), a broad approach is needed that couples molecular level details (electronic structure, molecular dynamics, etc.) with systems-level parameters (including rate constants, reaction energies, and yields). While specific problems in the broad field of catalysis spur novel questions, *an integrated and multi-capability infrastructure* for studying catalytic systems provides the greatest efficiency in the study of a wide range of problems. We propose a research campaign where unique nuclear magnetic resonance (NMR) capabilities, including both *in situ* and advanced *ex situ* ultra-high field NMR techniques, will be developed. Equal emphasis will be given to establishing high-level computational analyses at the molecular level to both explain and predict the structure and dynamics of molecules involved in catalytic reactions on surfaces, as well as how the temporal evolution of surface sites affects the catalytic activity. As this research campaign progresses, additional EMSL capabilities including the newly acquired He ion microscope will be leveraged to provide unprecedented details for understanding catalytic mechanisms and factors influencing the catalytic performance of a range of advanced materials.