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Title: Catalysis, Energy Storage, and Carbon Capture from a Computational Perspective

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This talk presents our efforts to understand catalysis, energy storage, and carbon capture from a computational perspective. The catalysis topic includes density functional theory studies of catalytic CO oxidation on cobalt oxide, gold cluster on a hydroxide support, and CO hydrogenation to ethanol. The topic of energy storage covers quantum chemical calculation of oxidation potentials of high-voltage electrolytes for Li-ion batteries and classical density functional theory of supercapacitors. In carbon capture, both chemical and physical interactions with carbon dioxide via liquid and framework separation media will be addressed from quantum chemistry, classical Monte Carlo, and atomistic molecular dynamics simulations. The challenge for computation in each topic will also be discussed.