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Density functional calculations in the automotive industry: Catalyst supports and hydrogen storage materials

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In my talk, I will describe some uses of density functional theory (DFT) calculations in the research laboratory at Ford, and particularly highlight work that was inspired by, or performed in collaboration with Ken Hass. I begin with a discussion of past work on γ-Al_2O_3 catalyst support materials, but also discuss the current main focus of our group's activities: hydrogen storage materials. Catalyst Supports: In current three-way automotive catalysts, precious metals are often supported by the phase of aluminum oxide known as γ-Al_2O_3. Despite the ubiquitous nature of this oxide in current automobile catalysts, and a considerable amount of effort expended to understand this material, many questions about the phase stability and even crystal structure of γ-Al_2O_3 remain. DFT calculations have made significant progress in unraveling these unanswered questions, allowing one to construct realistic models of the supported catalysts materials. Hydrogen Storage Materials: One of the major bottlenecks to the widespread use of hydrogen-fueled vehicles is the ability to store sufficient energy on-board to enable vehicle attributes acceptable to customers. I will give a general introduction to the topic of hydrogen storage, and a broad survey of the various classes of hydrogen storage technologies, and point out some pros and cons associated with each class. Currently known technologies have insufficient usable energy densities, and I will describe how DFT calculations are aiding the search for improved high density storage materials.