Driving Automotive Success with Dynamic Catalysis and Data Science

While the fleet of electric vehicles (EVs) is rapidly growing, the transition to fully electric mobility concepts critically depends on the available battery technology. In particular, solid-state batteries are the key enabling technology to produce reliable and safe EVs. Paramount to high performance solid-state batteries are solid-state electrolytes (SSEs) with high Li-ion mobility. However, the vast chemical design space for SSEs impedes trial-and-error approaches, but it provides ample room for data-driven discoveries. To this end, I will briefly discuss our approaches to use machine-learning for materials design and emphasize the need for suitable material representations (descriptors or fingerprints).

Despite the quickly growing market for EVs, fossil fuel powered vehicles with modern engine technologies will continue to dominate our roads for the near future. Low temperature combustion (LTC) diesel engines have higher fuel efficiency and produce less NO\textsubscript{x} and particulate matter (PM) compared to traditional diesel engines. Similarly, natural gas vehicles (NGVs) are relatively clean and emit less CO\textsubscript{2} compared to gasoline-powered cars. To leverage the benefits of these new engine technologies, they need to be paired with an advanced emission aftertreatment system. LTC engines require cold-start solutions and a low temperature diesel oxidation catalysts (DOC) that can cope with higher concentrations of CO and unburned hydrocarbons (HC). NGVs require modified three-way catalytic converters that can also oxidize methane; we refer to them as four-way catalytic converters (FWC).

To address cold-start NO\textsubscript{x} emissions, we study Pd-exchanged zeolites as passive NO\textsubscript{x} adsorbers (PNAs) to store NO\textsubscript{x} at low temperature and release it at higher temperature to a downstream DOC to adjust the NO/NO\textsubscript{2} ratio, followed by a reduction catalyst, which converts NO\textsubscript{x} to N\textsubscript{2}. We have also used computational screening for rapid catalyst discovery for DOC and FWC oxidation catalysts. Guided by our simulations, we have developed a dual-stage DOC prototype alloy catalyst and reactor configuration, which is able to meet the Department of Energy 150 °C challenge for CO oxidation in mixtures of CO/NO, CO/C\textsubscript{3}H\textsubscript{6}, CO/NO/ C\textsubscript{3}H\textsubscript{6}, and even CO/NO/C\textsubscript{3}H\textsubscript{6}/H\textsubscript{2}O. Similarly, we have optimized FWCs comprised of platinum group metals (PGM) and spinel oxides as dynamic oxygen storage materials.

Collectively, these significant, computationally driven advances are expected to accelerate the transition to modern and sustainable vehicle fleets.

**Tuesday, Oct. 5, 2021**
Lecture at 4:00 p.m.
1610 Engineering Hall