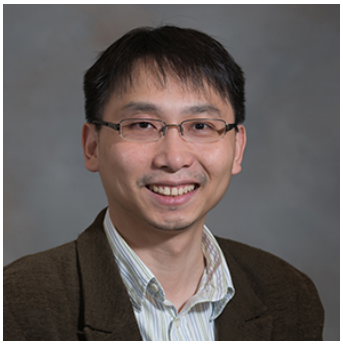

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Conversion of Carbon Dioxide to Cyclic Carbonates for Polymer Synthesis

Abstract.

The research goal of this proposal is to develop efficient ceria catalysts for recycling two categories of waste chemicals: carbon dioxide (CO_2) from fossil fuel combustion and bio-derived polyols such as glycerol from bio-diesel production, by transforming them into platform molecules to synthesize widely used polymers. The proposed chemical strategy is to combine CO_2 and polyols over defect engineered ceria catalysts to produce cyclic carbonates used in the production of polycarbonates and polyurethanes. A recent study reported the high conversion (>90%) of CO_2 and diols to cyclic carbonates using commercial ceria catalysts and replacing the use of lethally toxic phosgene and petroleum-based epoxides in the industrial synthesis. However, high temperature re-activation is required to recycle poisoned ceria catalysts and maintain their performance. Due to the insufficient understanding of the intrinsic properties of ceria catalyst (active sites and acid/base properties) and insufficient knowledge of intermediates for the CO_2 insertion reactions, utilization of ceria catalysts in molecular syntheses is limited in an industrial scale. The research objectives of this project are to obtain preliminary evidence for the roles of (1) ceria facets, (2) oxygen vacancy defects (OVDs), (3) additive dopant-induced lattice strain and defects, and (4) inorganic carbonate intermediate formed on ceria in the conversion of CO_2 and two polylol targets (glycerol and 1,2-propanediol) to the cyclic carbonates. Nanostructured ceria catalysts with different density of OVDs, facets, and dopants will be synthesized. The species and stability of carbonate intermediates formed on ceria catalysts will be probed by *in situ* infrared spectroscopy using a CO_2-pulse-probe technique. The evaluated catalytic results will be correlated to thermodynamic results from our modeling study to elucidate possible mechanistic reaction pathways and guide optimized catalyst design. The outcomes will be applied to study other chemical co-precursors to transform CO_2 into other classes of platform molecules.