Accelerating Catalyst Design for Selective Ethane Oxidative Dehydrogenation

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Project Summary

Selective ethane oxidative dehydrogenation (EODH) to ethylene is a critical chemical transformation as ethylene is a widely used chemical building block. Industrially, ethylene is produced either through high temperature steam cracking or through dehydrogenation over Cr or Pt based catalysts. Both processes have significant disadvantages, with the former being highly energy intensive and the latter resulting in significant coke formation on the catalyst surfaces. One class of catalyst materials showing promise here are transition metal oxides. The use of an oxide catalyst changes the overall reaction from dehydrogenation to EODH, thereby shifting the overall reaction enthalpy and lowering the necessary temperature. However, the challenge remains to prevent undesired side reactions, including excessive C-H and C-C scission and C-O formation. The overall goal of this proposed research is to tackle such challenges by enabling the science-guided design of transition metal oxide catalysts for EODH by mapping the structure, energetic profile, and reactivity of a range of promoted NiObased mixed metal oxide (M-NiO) surfaces, including promoter type, facet, metal and oxygen defects, and degree of hydroxylation effects. Our approach utilizes a combination of density functional theory calculations and transition state theory microkinetic modeling to determine the dominant surface structures present under working conditions, identify the most favorable potential energy surface, and predict the overall catalytic performance. Taken together, we expect this work to establish crucial, fundamental connections between promoter properties, working catalyst structure, nanoscale energetics, and catalytic performance, thus setting a critical foundation for the rapid and rational design of EODH catalysts.