Quantum Theory Prediction of Anionic Metal Oxide Catalyst Efficiency for Methane-to-Methanol Conversion

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Standard oil well and fracking site operations typically burn off large amounts of methane due to the high costs associated with its utilization. On-site conversion of methane to liquid methanol, however, could help circumvent this practice by dramatically lowering the cost of transportation to facilities where it can be made into useful commodities. That said, previous attempts to develop a viable on-site conversion strategy have proven ineffective largely due to cationic catalysts not only activating the C-H bond of methane, but also the weaker C-H bond of methanol, leading to over-oxidized byproducts. As such, I hypothesized that an anionic catalyst would not only efficiently convert methane to methanol, but also quickly separate produced methanol from the catalyst, limiting the creation of byproducts. To examine this, I tested an anionic catalyst with the proper ligand by identifying the reaction mechanism species for two spin states of copper, nickel, and cobalt and calculating the energies using density functional theory. I then evaluated both the energy kinetics to analyze efficiency and the reactant selectivity to determine the strength of its interaction with methanol. Importantly, and directly supporting my hypothesis, I found that the copper doublet outperformed other metals, avoided the release of methyl radicals, and favored producing methanol rather than unwanted byproducts. In summary, methane is a highly problematic substance, not only because of its potent greenhouse effects, but also due to the $10 billion of economic damages it causes per year in the U.S. alone, and the work presented here strongly suggests anionic catalyst utilization can significantly improve efforts to develop a viable strategy for on-site conversion of methane to liquid methanol.

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