Oxidation of Methane to Methanol on a Porphyrin-Supported Copper Oxide Nanoparticle

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During the last decade, natural gas production in the United States has grown continuously, and it is predicted to grow even more rapidly during the coming years. New opportunities for energy efficiency and resource conservation provided by the natural gas boom are driving efforts to overcome the catalytic challenge of selectively transforming natural gas components into more valuable chemicals. The catalytic transformation methane to methanol under ambient conditions is one of the grand challenges towards harnessing the abundant natural gas supply into a more useful feedstock. We have performed a density functional study of the atomic layer deposition growth of a copper metal oxide nanoparticle supported on a porphyrinic substrate and evaluated its performance for the oxidation of methane to methanol. We explored different oxidants and reaction pathways, as well as the effect of a hydrogen pre-treatment on the nanoparticle structure and catalytic activity.