Computational Studies on Fischer-Tropsch Catalysis in Astrophysical Environments

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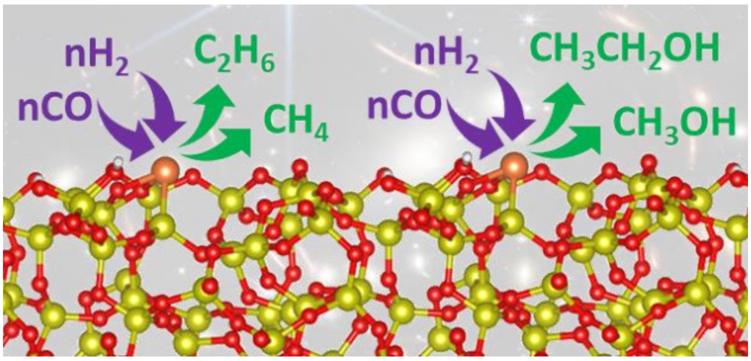
The formation of Solar-like planetary systems is a complex process where not only physical changes occur but also increasing molecular complexity is observed. This gives rise to a rich chemical diversity and complexity of gas-phase molecular species in different astrophysical environments.[1] However, chemistry in the gas-phase at such low densities and temperatures is difficult, and not all the molecules observed can be formed at this state. The presence of interstellar grains (i.e., submicron-sized solid-state particles ubiquitously present in space) is especially important for the synthesis of molecules that cannot form in the gas phase in the abundance required to satisfy observations. Interstellar grains are advocated to infer catalytic effects. However, such a "catalytic role" is associated with enhancement of the encounter rate of the reactive species on the grain surface due to adsorption and diffusion, and the capability of the grains to dissipate the energy excess of largely exothermic reactions. It is not associated with the provision of lower activation energy pathways with naturally enhanced reaction rates.[2] Nevertheless, different materials that can exhibit true catalytic properties are present in interstellar environments. Refractory grains containing space-abundant transition metals (such as Fe and Ni) are the perfect candidates to perform as heterogeneous catalysts.[3]

In this present work, we report mechanistic insights on the catalytic formation of short chain alcohols (e.g., methanol and ethanol), aldehydes (e.g., formaldehyde and acetaldehyde) and short chain hydrocarbons (e.g., methane and ethylene) in interstellar conditions through the Fischer-Tropsch process. The reaction proposed here is catalysed by single-atom Fe containing silica surfaces (SiO_2). Beyond mechanistic descriptions, kinetic data are also provided to corroborate the feasibility of this process under corresponding interstellar temperature conditions. The evidence of astrocatalysis opens a completely new spectrum of synthetic routes which are starting points for triggering chemical evolution in space.



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[2] J. A. Nuth III et al. Meteorites Early Sol. Syst. II. **147**, 147–167, (2006).
[3] W. F.Bottke et al. Nature, **485**, 78–81, (2006).