Haber-Bosch at the atomic scale

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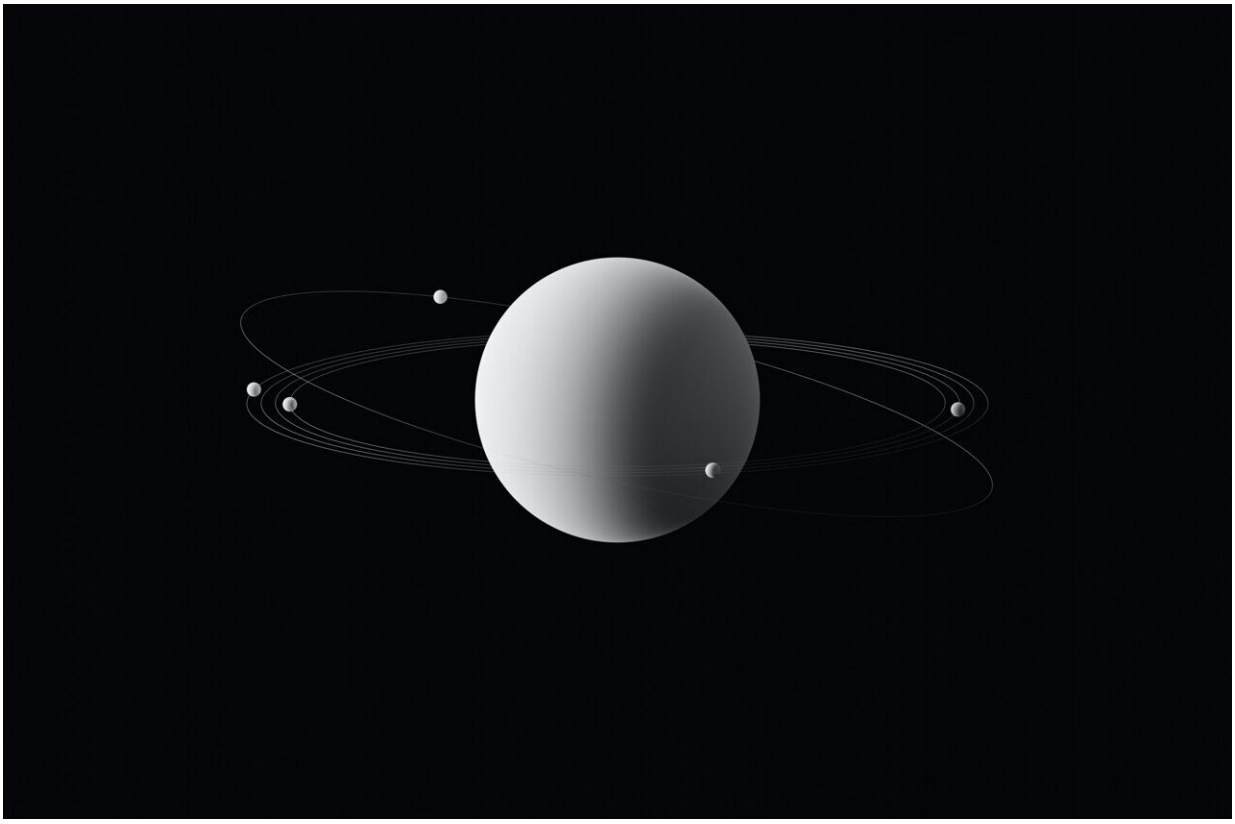

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Industrial production of NH_3 has been performed by the Haber-Bosch process for more than 100 years, in which dissociation of N_2 feedstock molecules promoted by alkali atom co-catalyst is thought to be the rate limiting step. The Haber-Bosch synthesis consumes 1% of the world's total energy consumption, and accounts for 1.4% of the global CO_2

emissions. Therefore, the atomic scale insights into the K atom-N_2 molecule interactions on metal substrates and specifically, the alkali atom promotion chemistry, has global significance.

Researchers at the University of Pittsburgh, together with theoretical collaborators at the University of Science and Technology of China have investigated the Haber-Bosch catalysis precursor at the atomic scale.

In research article to be published in *Cell Reports Physical Science* on April 21, 2022, the researchers, led by Hrvoje Petek at the University of Pittsburgh, were able to directly observe at the atomic scale by scanning tunneling microscopy the N_2 adsorption, their collective interactions, and tunneling electron-induced N_2 desorption processes that are related to the alkali promotion of NH_3 synthesis.

The dominant pairwise interaction between the K and N_2 is an electrostatic, two-center, Coulomb attraction, where charge transfer from K to N_2 weakens the N_2 molecule bond towards its dissociation in the Haber-Bosch synthesis. The K-N_2 interactions interpreted through density functional theory are in agreement with the experimental observations.

The studies reveal the primary interactions, as well as the onset of correlated complexity that defines the alkali atom promotion of catalytic chemistry.

More information: Chao Zhang et al, Imaging a Haber-Bosch catalysis precursor at the atomic scale, *Cell Reports Physical Science* (2022). DOI: 10.1016/j.xcrp.2022.100865

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