Deciphering the operando mechanism of Haber-Bosch process

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The Haber-Bosch synthesis of ammonia (NH_3)[1], a cornerstone of modern industry, was a defining invention of the twentieth century. Despite its maturity, the catalytic mechanism at its operating conditions remains poorly understood. Debates persist over the active catalytic phase and the rate-limiting step[2-10]. A major limitation has been that most studies are performed at low pressures at low pressures (~1 bar), which are not representative of industrial *operando* conditions (~200 bar). To bridge this "pressure gap," we have employed machine learning interatomic potentials to perform large-scale, *ab initio*-accurate simulations at *operando* conditions. This talk will present our latest computational insights into the nitrogen reduction pathway under realistic Haber-Bosch environments.

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