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Explaining The Weak Catalyst Dependence In Low-Pressure Plasma Synthesis of Ammonia GIORGIO NAVA, SHARMA YAMIJALA, BRYAN WONG, LORENZO MANGOLINI, University of California Riverside — Low-temperature plasmas have recently emerged as possible pathway for decentralized nitrogen fixation, a promising alternative to the Haber Bosch process. While several reports confirm that it is possible to produce ammonia using a plasma, these works also highlight a weak dependence on the catalyst material of choice. This last aspect is not consistent with established models. In this contribution, we present the results of a combined experimental/computational investigation on the formation of ammonia in a low-pressure hydrogen-nitrogen discharge. In good agreement with previous literature, we observe that the degree of nitrogen fixation has a weak dependence on the catalyst of choice. Ab-initio Born Oppenheimer molecular dynamics simulations are deployed to elucidate the origin of this behavior. It is found that ammonia production follows an Eley-Rideal mechanism. The weak difference in the ammonia production yield displayed by the materials stems from their different ability to store atomic nitrogen at their surface. The atomic hydrogen flux to the catalyst surface, characterized via optical emission spectroscopy, largely exceeds that of atomic nitrogen, making the ammonia production yield mass transport limited by the flux of atomic nitrogen.

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