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Towards Accurate Reaction Mechanisms for N_2-H_2 Low-Temperature Plasma Simulations

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We live in an era shaped by groundbreaking technologies, but there was a time when tools like *ChatGPT* or even the personal computers we now rely on to search the web did not exist. These innovations didn't simply appear; they are the result of collective effort and years of development to reach the sophistication we see today. In the context of plasma physics, it is tempting to assume we already possess precise plasma simulation capabilities, but the reality is far from complete. This study positions itself at the frontier of plasma research, striving to advance the state of the art. By contributing to one of the most sophisticated plasma simulation tools, the LisbOn KInetics (LoKI) code developed by the PSI.COM group at the Instituto de Plasmas e Fusão Nuclear (IPFN), and by refining reaction mechanisms pivotal for simulation accuracy, this work aims to push the boundaries of plasma modeling. This includes validating and simplifying these mechanisms using machine learning and conducting experimental diagnostics through a dedicated measurement campaign at the Laboratoire de Physique des Plasmas (LPP) in Paris. Focused on nitrogen-hydrogen (N_2-H_2) plasmas, the research investigates the kinetic pathways of ammonia (NH_3) synthesis, offering critical insights for scalable production of sustainable fertilizers, hydrogen-based energy storage, alternative fuels, and advancing the broader plasma science community.

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