Highlights

RESEARCH AREA 1 - Superconductors and Innovative materials for Energy and Environment - 2024

Molecular hydrogen in the N-doped LuH_3 system as a possible path to superconductivity

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The discovery of superconductivity under ambient or near-ambient conditions would represent a long-sought scientific milestone, with important implications for fundamental science and future technologies. The recent observation of high-temperature superconducting phases in compressed hydrides has renewed optimism that this goal may be closer than ever. Yet, a major challenge remains: hydride synthesis under extreme conditions often favors the formation of multiple metastable and disordered phases, leading to experimental observations that are often difficult to reproduce and making their structural identification highly difficult and often very controversial.
In this work, we address these issues by considering N-doped LuH_3 as a prototypical complex hydride system. Through machine-learning-accelerated force-field molecular dynamics, we uncover the formation of H_2 molecules stabilized at ambient pressure by nitrogen impurities. Most importantly, we demonstrate that this molecular phase plays a key role in enabling a dynamically stable superconducting state at low temperature and ambient pressure.
Beyond providing a microscopic framework to interpret debated results in lutetium hydrides, our findings reveal that this molecular phase plays a pivotal role in the emergence of a dynamically stable, low-temperature, ambient-pressure superconductivity. The potential to stabilize hydrogen in molecular form through chemical doping opens up a novel avenue for investigating disordered phases in hydrides and their transport properties under near-ambient conditions.

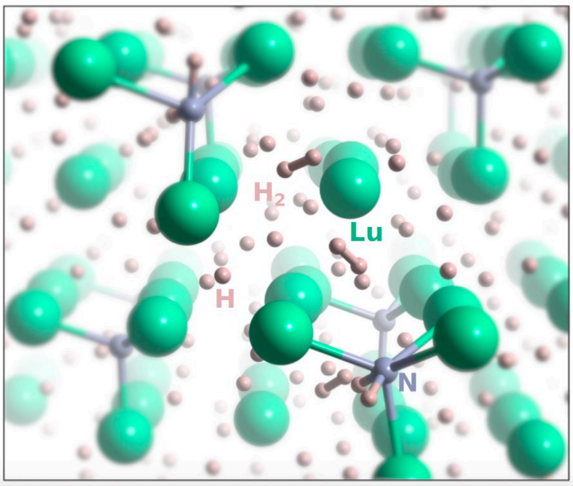

Fig. 1: Snapshot of the MLFF-MD showing the disordered phase with H-H and N-H bonds.