Contribution ID: **14** Type: **not specified**

DFT and AIMD Investigation of Hydrogen Storage in Alkali Metal Hydrides XH (X=Li, Na, and K)

Tuesday, 18 November 2025 10:45 (15 minutes)

This study employs first-principles density functional theory (DFT) calculations to
examine the hydrogen storage capacity of alkali metal hydrides (XH, where X = Li, Na, and K). We systematically examine the structural, mechanical, dynamical, electronic, and thermodynamic properties of these hydrides, along with key hydrogen storage metrics, such as gravimetric and volumetric capacities, and desorption temperatures. The results demonstrate that all of the investigated hydrides are thermodynamically stable. LiH demonstrates the highest performance among them, with gravimetric and volumetric capacities of 12.68 wt% and 104.13 g.H 2 /L, respectively. In contrast, NaH and KH have lower gravimetric capacities of 4.20 wt% and 2.51 wt%, respectively, and lower volumetric capacities of 59.32 g.H 2 /L and 36.16 g.H 2 /L, respectively. The estimated desorption temperatures are 612.40 K for LiH, 315.81 K for NaH, and 396.58 K for KH. Ab initio molecular dynamics (AIMD) simulations confirm the thermal stability of these hydrides at room temperature. Overall, alkali metal hydrides show promising potential as hydrogen storage materials.

Primary author: Ms OUHENOU, Hakima (Laboratory of Research in Physics and Engineering Sciences, Sultan Moulay Slimane University, Polydisciplinary Faculty, Beni Mellal, 23000, Morocco.)

Co-authors: ABBASSI, Abderrahman; MANAUT, Bouzid; FATIHI, Hmad; AGOURI, Mohamed; TAJ, Souad

Presenter: Ms OUHENOU, Hakima (Laboratory of Research in Physics and Engineering Sciences, Sultan Moulay Slimane University, Polydisciplinary Faculty, Beni Mellal, 23000, Morocco.)

Session Classification: Tuesday Morning II

Track Classification: AfPS