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Faculty of Exact Sciences

The First International Conference of Chemistry and Physics:
Two disciplines, a unified vision of matter. 1st-ICCP 2025
December 14-15, 2025. Constantine, Algeria

CERTIFICATE OF ATTENDANCE

The scientific committee of 1st-ICCP 2025 certifies that:

SAADOUN Samira

has attended the congress with a poster presentation entiteled:

First principles investigation of the structural and electronic properties of Na1-xLixMgH$_3$ hydrides for enhanced solid-state hydrogen storage

Co-authors are respectively: ***T. Ghellab, H. Baaziz & Z. Charifi***

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First principles investigation of the structural and electronic properties of $Na_{1-x}Li_xMgH_3$ hydrides for enhanced solid-state hydrogen storage

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Density Functional Theory (DFT) is implemented in the wien2k code are investigates the hydrogen storage properties of $Na_{1-x}Li_xMgH_3$ hydrides (x = 0, 0.25, 0.5, 0.625, 0.75,1). Results show that lithium substitution increases hydrogen storage, with gravimetric and volumetric capacities increasing from 6.00 wt% and 90 gH_2/l (x = 0) to 8.82 wt% and 214 gH_2/l (x = 1), surpassing U.S. DOE aims (5.5 wt% and 40 gH_2/l) The theoretical specific capacity improves from 1590 to 2331 mAh/g. A phase transition at x = 0.625 (from orthorhombic *Pnma* to trigonal *R3c*) improves hydrogen packing. Among dehydrogenation pathways, we looked at a few different ways to dehydrogenate, and Pathway 7 is the best. The desorption temperatures drop from 256 K to 145 K as the Li content grows increased. Research on cohesive and binding energy shows that adding lithium makes the structure more stable and the atomic interactions stronger. All of the compositions are insulators with significant band gaps. When the amount of Li goes up, the band gaps become bigger, going from around 3.45 eV to about 6.77 eV. These findings underscore the promise of $Na_{1-x}Li_xMgH_3$ hydrides as efficient and stable substances for solid-state hydrogen storage.

References:

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