

***In Situ* Study of NaAlH₄ Confinement in Mesoporous Carbon Black for Hydrogen Storage**

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Solid-state hydrogen storage in complex metal hydrides, such as sodium alanate (NaAlH₄), is considered an efficient hydrogen storage method for enabling a hydrogen economy. However, high operating temperature and H₂ pressure requirements remain crucial obstacles to practical applicability. Nanoconfinement in porous media is one way of tackling these obstacles. For this purpose, confinement of NaAlH₄ inside a mesoporous carbon black with high NaAlH₄ content (50-90 wt%) is presented. These composites were prepared via ball milling and studied with temperature-programmed dehydrogenation, ex-situ powder X-ray diffraction, and dehydrogenation/hydrogenation cycling.¹ Furthermore, the deuterated 60 wt% NaAlD₄/carbon black composite was studied *in situ* via neutron powder diffraction over multiple decomposition/deuteration cycles performed at different conditions.²

Considerable lowering of dehydrogenation temperatures down to near-ambient, ~373 K, is shown, which is significant compared to bulk alanate's ≥ 456 K. In addition, partial hydrogenation is shown under 6 MPa of H₂ pressure and at 423 K. The Na₃AlD₆ \leftrightarrow NaD transition is shown to be almost entirely reversible at the applied low deuterium pressures of ≥ 2 MPa *in situ* via neutron diffraction of the deuterated sample. All the different physical characterization methods have given insight into the fundamental processes driving the H₂ release and uptake and the changes in crystalline phase composition. The strong effect of even low additions of mesoporous carbon black as a supporting scaffold material on the capability to store H₂ reversibly is elucidated and analyzed in-depth.

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References

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