

New Directions for Hydrogen Storage: Sulphur Destabilized Sodium Aluminium Hydride

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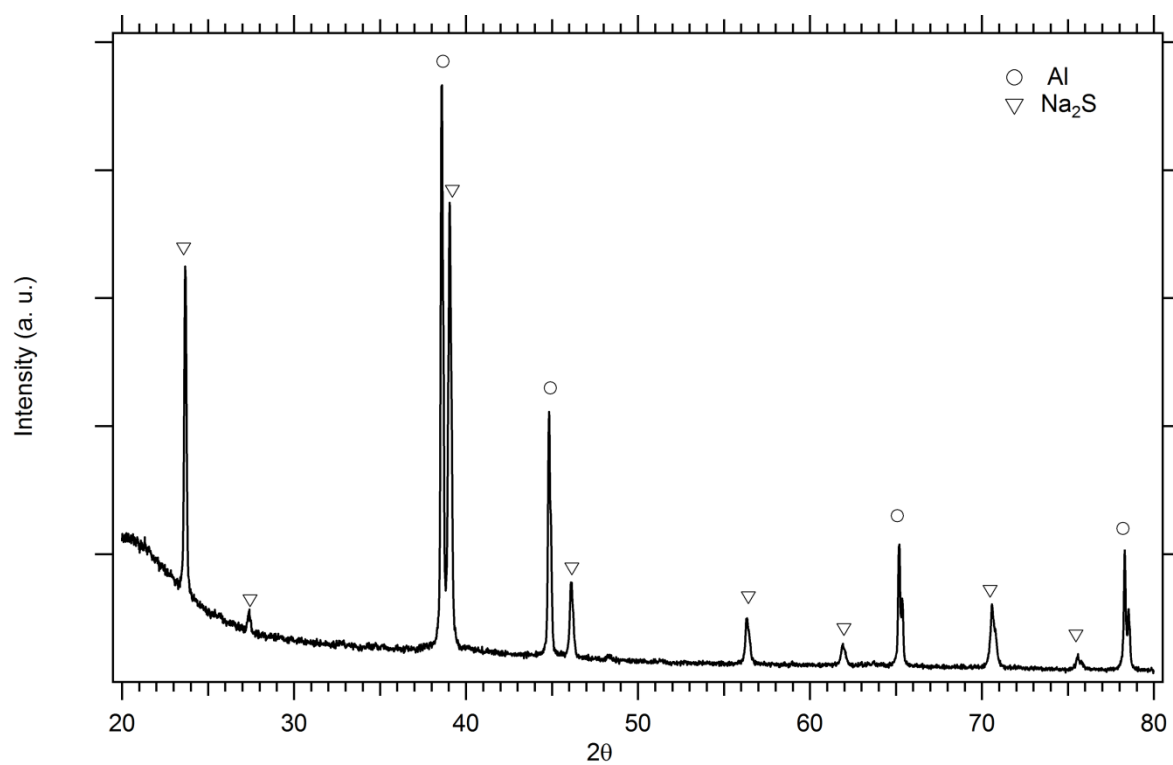


Figure S1. Laboratory XRD ($\lambda = 1.5406 \text{ \AA}$) of NaAlH₄-Al₂S₃ after desorption at 375 °C, measured on a Bruker D8 instrument.

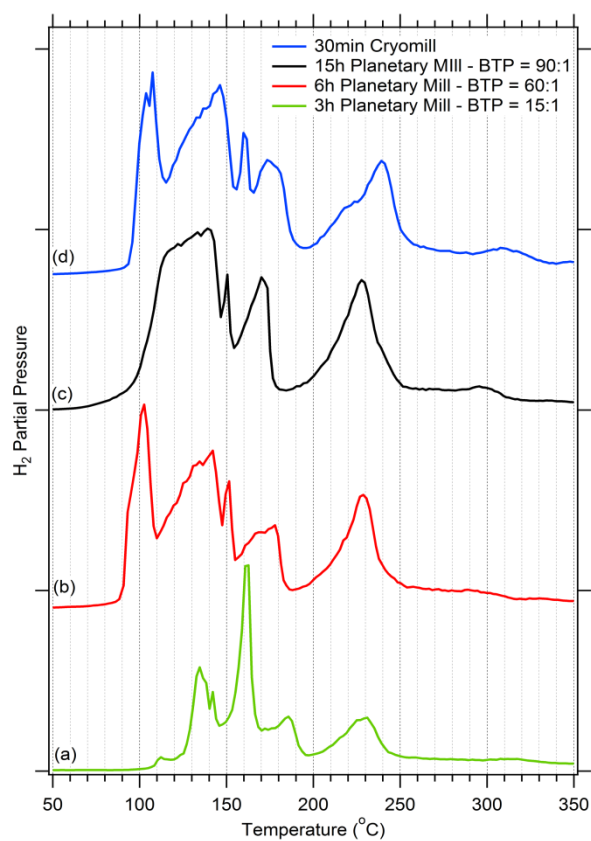


Figure S2. Temperature Programmed Desorption of NaAlH_4 - Al_2S_3 after ball-milling for (a) 3 h at a BTP = 15:1, (b) 6 h at a BTP = 60:1, (c) 15 h at a BTP = 90:1, and (d) 30 minute cryomilling. Heating rate = $1^\circ\text{C}/\text{min}$.

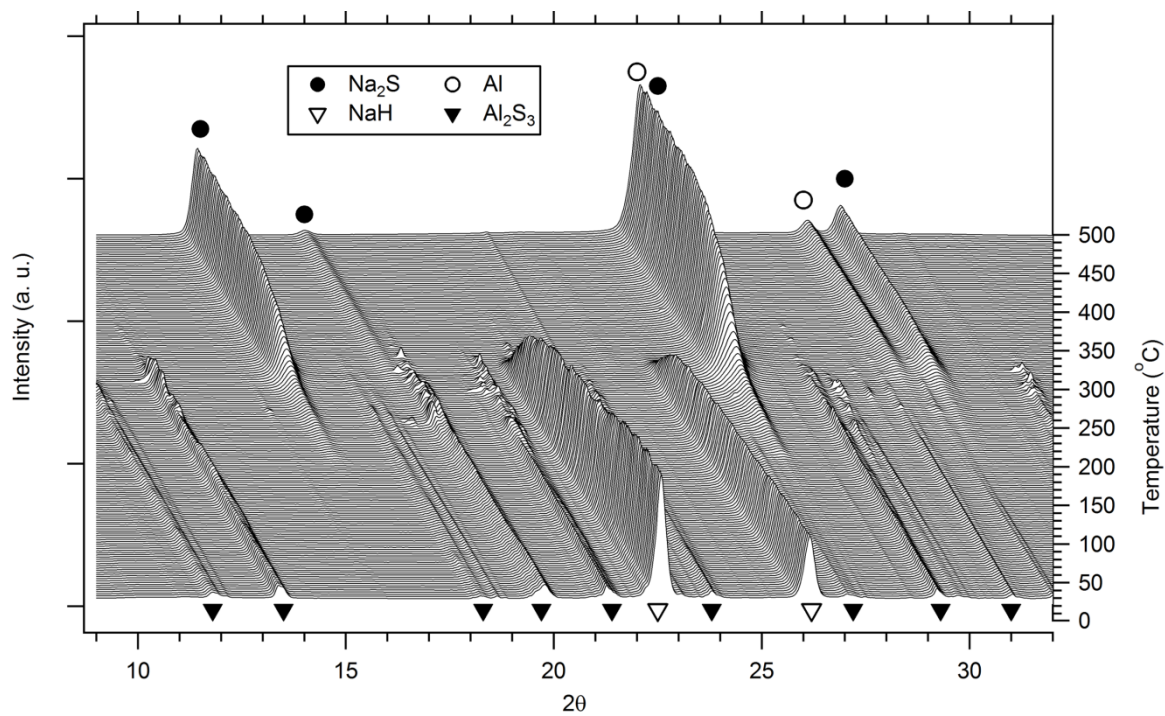


Figure S3. *In-situ* SR-XRD ($\lambda = 1.10113 \text{ \AA}$) of $\text{NaH-Al}_2\text{S}_3$ desorbed under vacuum at a heating rate of $5^\circ\text{C}/\text{min}$.

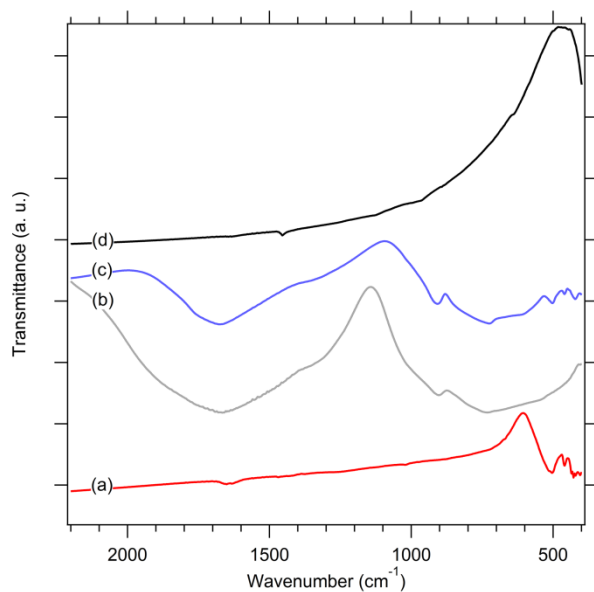


Figure S4. Fourier Transform Infra-Red spectroscopy pattern of (a) pure Al₂S₃, (b) pure NaAlH₄, (c) NaAlH₄-Al₂S₃ after ball-milling for 6 h and (d) pure Na₂S.

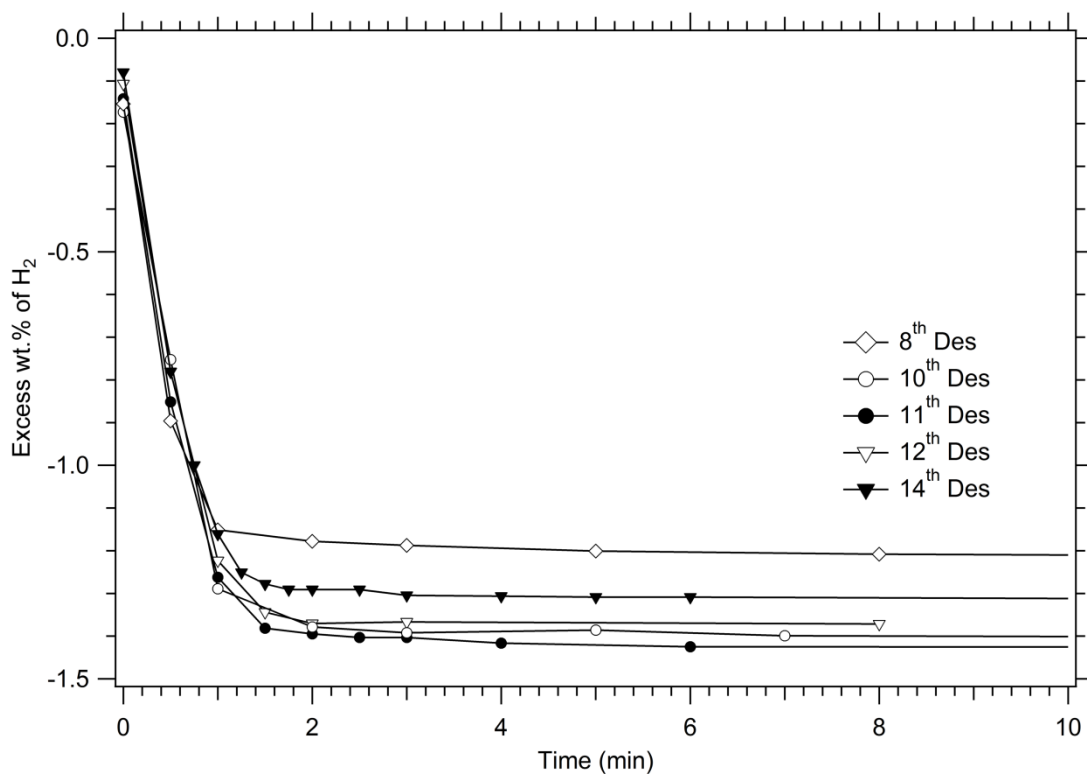


Figure S5. H₂ desorption from NaAlH₄-Al₂S₃ over multiple cycles at 300 °C. Desorption was performed against a H₂ back-pressure of between 63 and 76 bar.

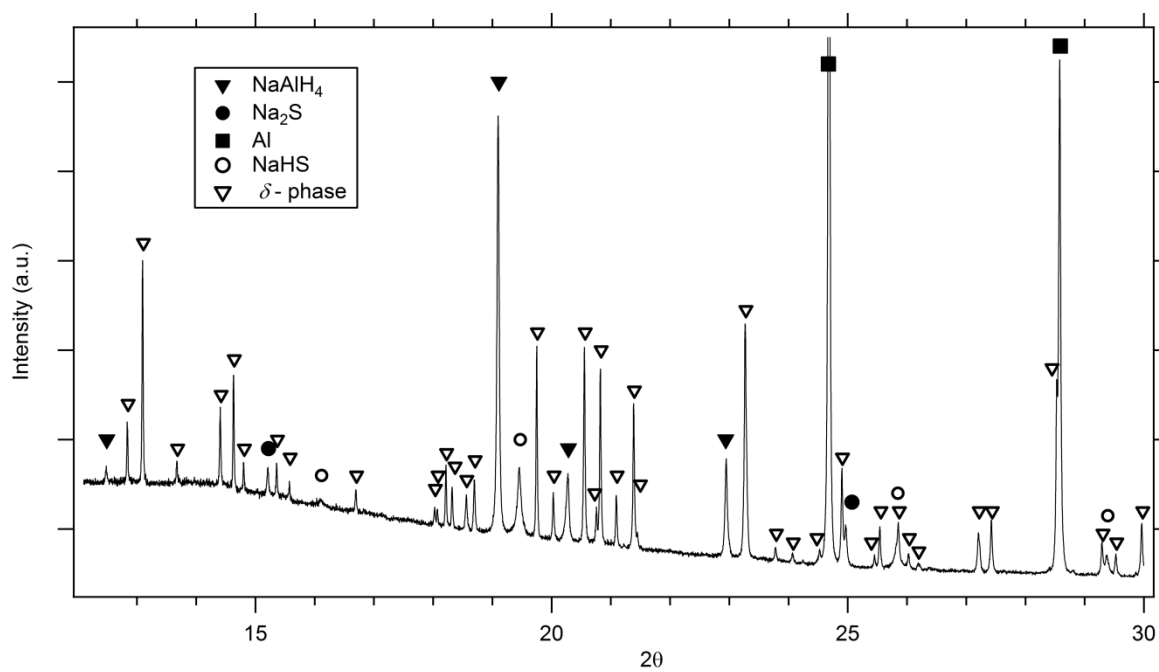


Figure S6. *Ex-situ* SR-XRD of $\text{NaAlH}_4\text{-Al}_2\text{S}_3$ decomposed under vacuum at 375 °C followed by hydrogenation at 300 °C under 282 bar H_2 pressure.