Electronic Supporting Information (ESI)

Metal hydride-based materials towards high performance negative electrode for all-solid-state lithium-ion batteries

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Experimental Section

Sample preparation and battery assembly:

The MgH₂ (98%, Alfa Aesar) was used as received and c–MgH₂ was synthesized by ball–milling 99 mol% of MgH₂ and 1 mol% of Nb₂O₅ (99.5%, Sigma–Aldrich) for 20 h. The composite electrodes were synthesized by mixing c–MgH₂, LiBH₄ (\geq 95%, Sigma–Aldrich) and acetylene black with ball–milling method at a weight ratio of 4:3:3. The powder electrode materials were then loaded into stainless steel vessels with 15 mm inner diameter and pressed into tablet together with the LiBH₄ solid electrolyte at 160 MPa. Afterwards, a lithium metallic disk was placed on the LiBH₄ electrolyte as counter electrode. Finally, these pellets were placed into the experimental cells (Toyo System Co.) sealing with PTFE O–rings for battery testing. All procedures were done in the Ar filled glove boxes.

Measurements and Characterization:

The thermal analysis was performed by a thermogravimetry with differential thermal analysis equipment (TG-DTA, Rigaku, TG8120) at a heating rate of 5 °C min⁻¹. The discharge–charge property was performed with galvanostat (HJ–SM8, Hokuto Denko Co.) between 0.3 and 1.0 V (vs Li⁺/Li) at the current densities of 100–3200 mA g⁻¹ at 120 °C. The obtained discharge/charge capacities were calculated based on the weight

of MgH_2 only. The structural characterization was conducted by powder XRD measurement (RINT2000, Rigaku) using Cu K α radiation at room temperature. The samples for XRD were protected with polyimide film to avoid the oxidation and the adsorption of water during measurement.

Figures



Fig. S1 The TG–DTA result of the MgH_2 –LiBH₄ composite heating up to 275 °C. The peak at 115 °C on DTA profile is corresponding to the phase transition of LiBH₄.



Fig. S2 The XRD result of MgH_2 -LiBH₄ composite electrode charged to 2.0 V.