Supplementary Materials

A potential hydrogen isotope storage material Zr_2Fe: deep exploration on phase transition behaviors and disproportionation mechanism

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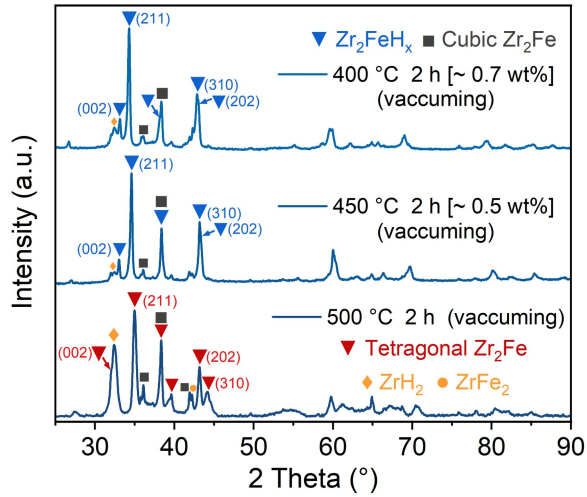


Figure 1. XRD patterns of dehydrogenated Zr_2Fe samples after dehydrogenation at different conditions.

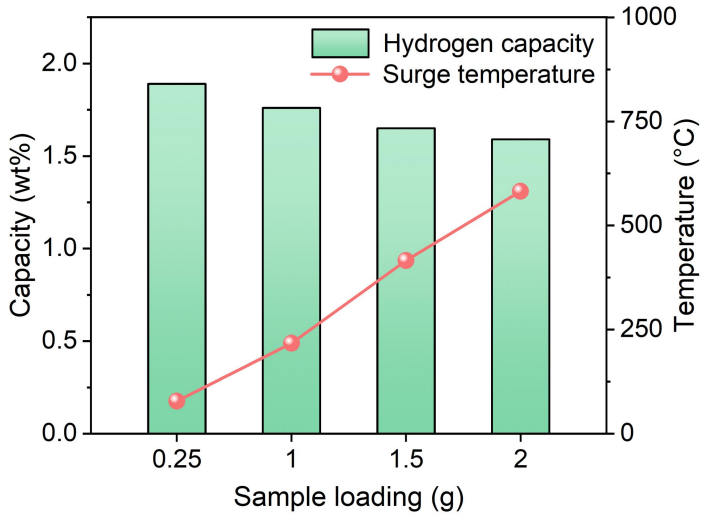
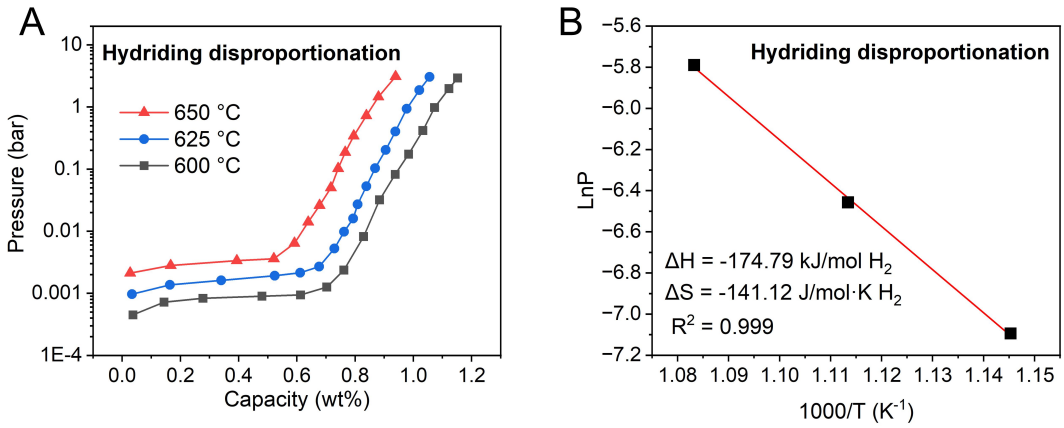


Figure 2. The relationship between the hydrogen capacity (initial pressure: 1 bar) of Zr_2Fe, the surge temperature and sample loading.



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39 **Figure 3.** Hydriding disproportionation PCT curves of Zr_2Fe samples at 600, 625,

40 650°C (A) and their corresponding Van't Hoff plots (B).

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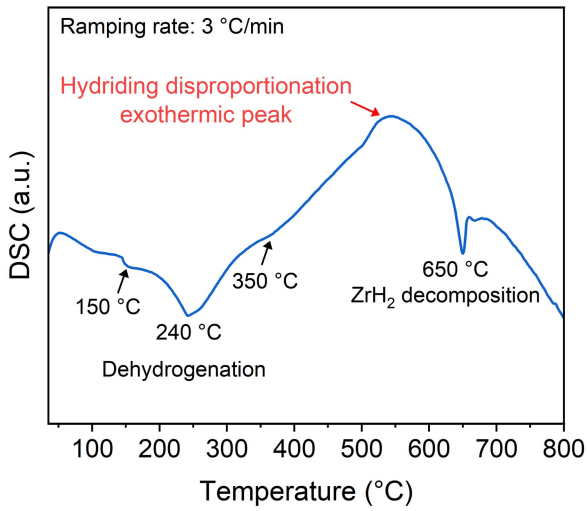

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43 **Figure 4.** DSC curve of the Zr_2FeH_5 at ramping rate of 3 °C/min.

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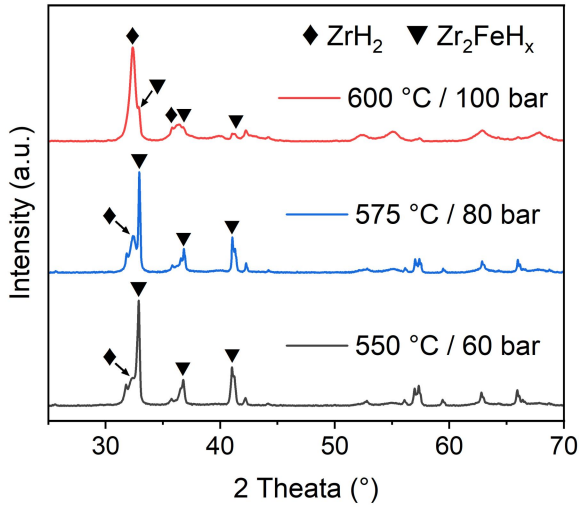

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48 **Figure 5.** XRD patterns of Zr_2FeH_5 after being kept at a specific high temperature and

49 pressure for 2 h.

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51 **Table 1. Lattice parameters of Zr_2Fe, Zr_2FeH_2 and Zr_2FeH_5**

Phase	Lattice parameters (Å)			Volume (Å^3)	Average Expansion rate per H
	a	b	c		
Zr_2Fe	6.266	6.266	5.738	225.3	4.12%
Zr_2FeH_2	6.640	6.677	5.502	243.9	3.37%
Zr_2FeH_5	6.903	6.903	5.637	268.6	

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