Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Thermochemical Energy Storage Performance of Zinc Destabilized Calcium Hydride at High-Temperatures†

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| | Predicted reaction | Theoretical $H_2$ wt% |
|---|---|---|
| 1 | $3CaH_2 + Zn \leftrightarrow Ca_3Zn + H_2(g)$ | 3.15 |
| 2 | $5CaH_2 + 3Zn \leftrightarrow Ca_5Zn_3 + H_2(g)$ | 2.47 |
| 3 | $CaH_2 + Zn \leftrightarrow CaZn + H_2(g)$ | 1.87 |
| 4 | $CaH_2 + 2Zn \leftrightarrow CaZn_2 + H_2(g)$ | 1.16 |
| 5 | $CaH_2 + 3Zn \leftrightarrow CaZn_3 + H_2(g)$ | 0.84 |
| 6 | $CaH_2 + 5Zn \leftrightarrow CaZn_5 + H_2(g)$ | 0.54 |
| 7 | $CaH_2 + 11Zn \leftrightarrow CaZn_{11} + H_2(g)$ | 0.26 |
| 8 | $CaH_2 + 13Zn \leftrightarrow CaZn_{13} + H_2(g)$ | 0.22 |

**Table S1.** Theoretical predictions of possible reaction between $CaH_2$ and Zn and corresponding $H_2$ wt. %.

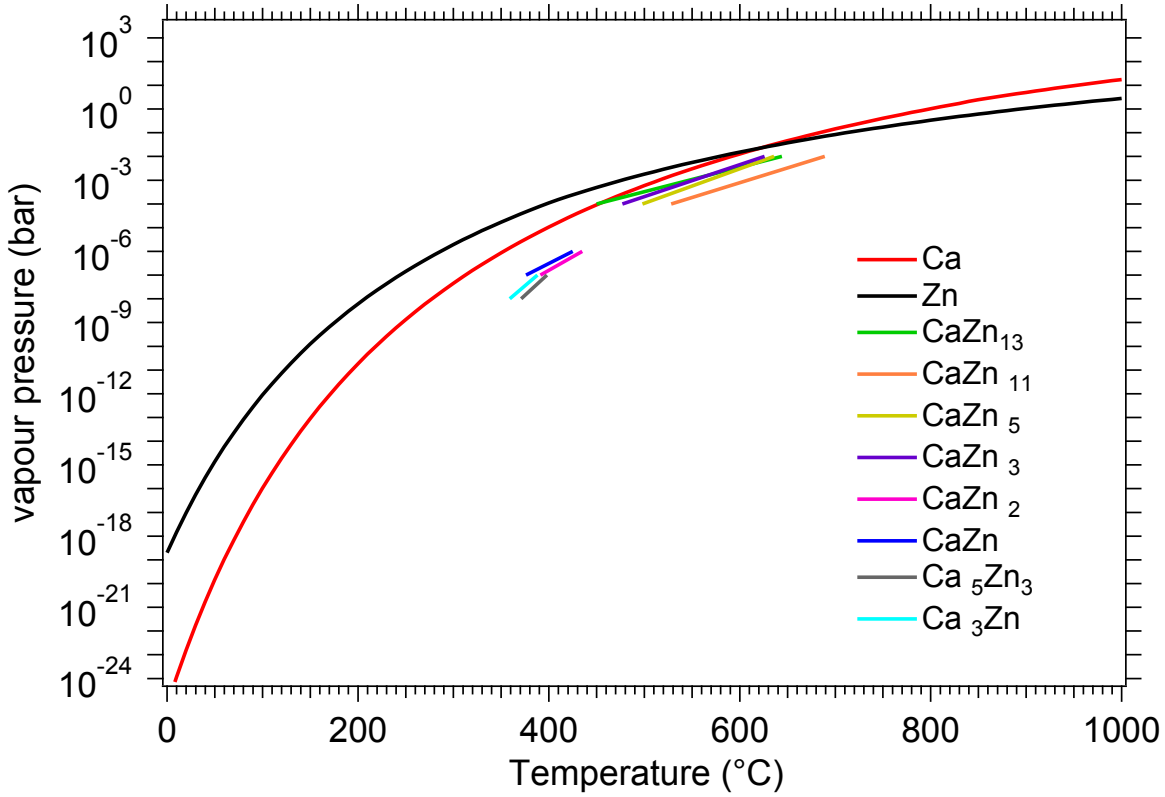



**Fig. S1**. Vapour pressure curves for pure Ca and Zn and calcium zinc alloys as a function of temperature.[1-4]

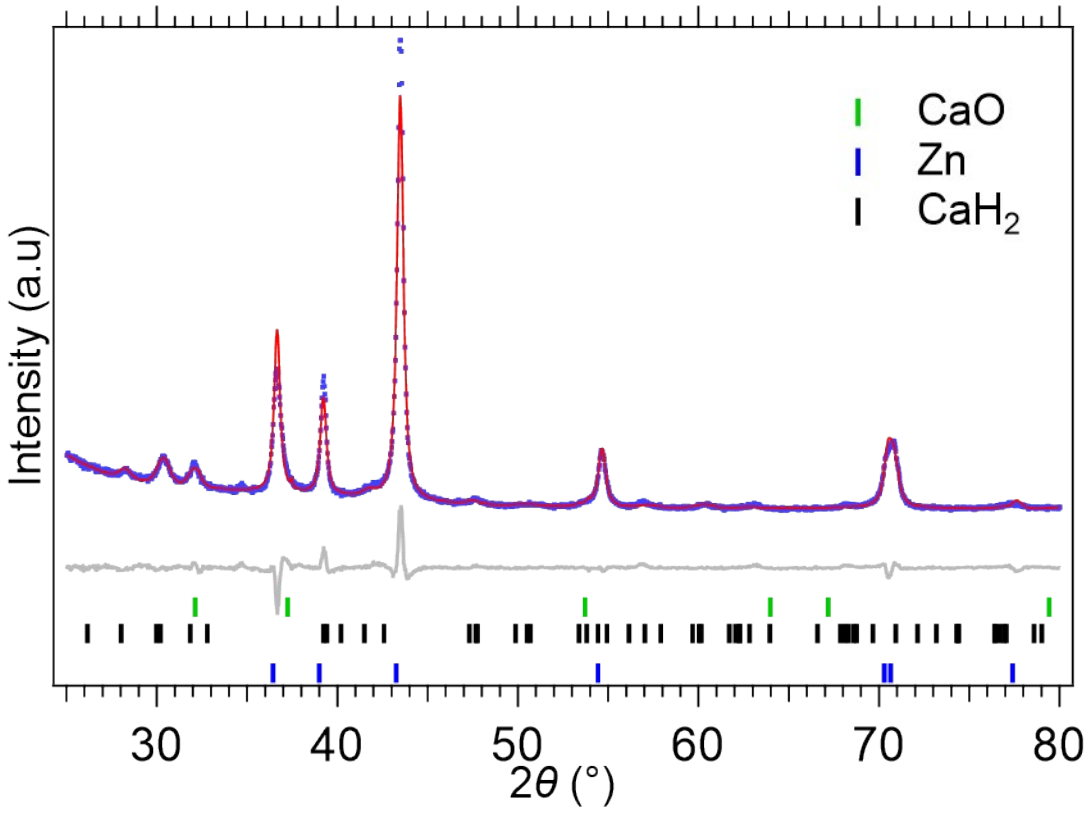



**Fig. S2** Rietveld refinement of the diffraction pattern for CaH2-3Zn system after ball milling (Cu Kα radiation ($\lambda$ = 1.5418 Å).

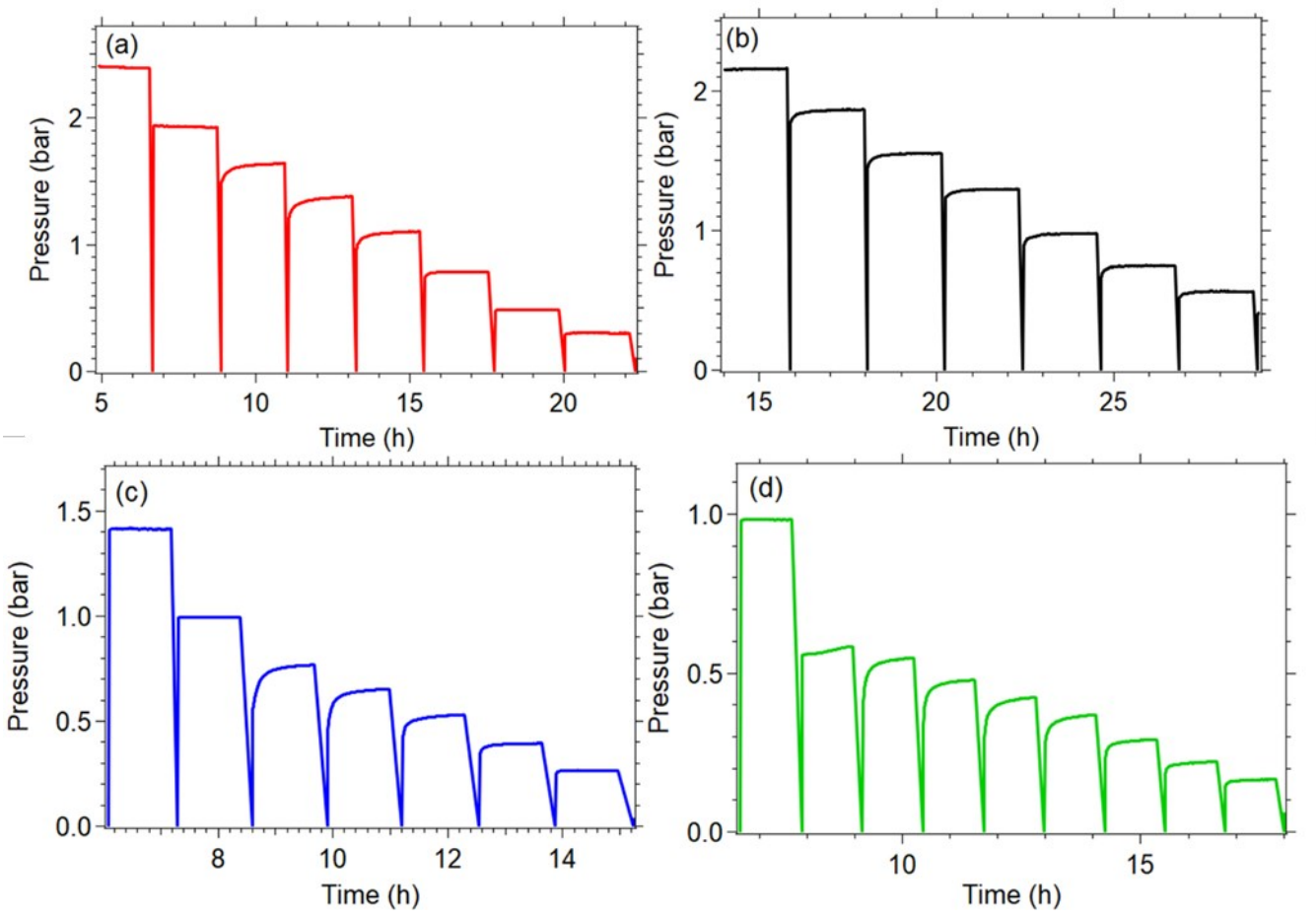
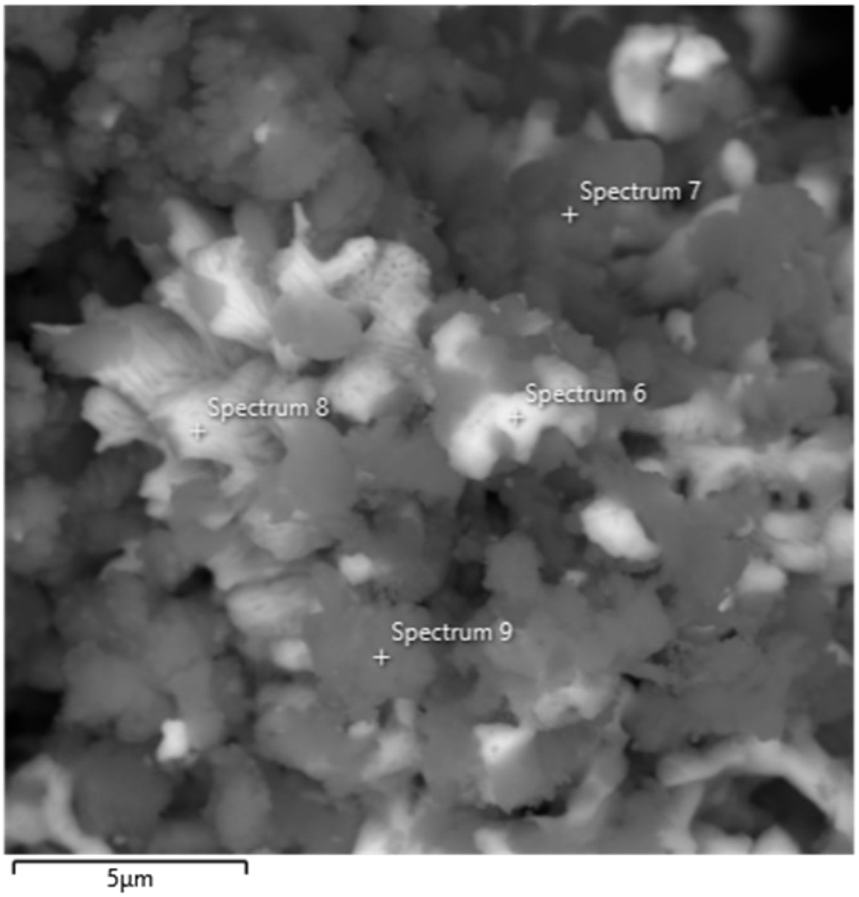



**Fig. S3** Equilibrium pressure curves of PCI performed at (a) 614 °C (b) 600 °C (c) 580 °C and (d) 565 °C with 3 h desorption step sizes.



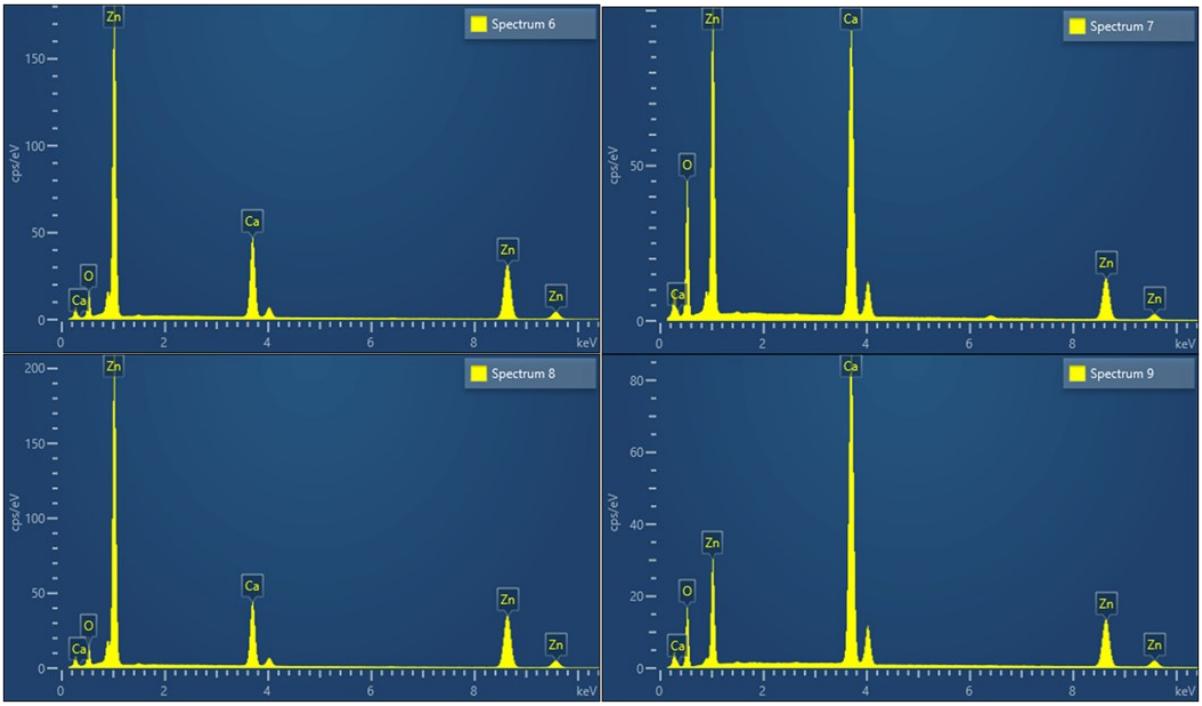



**Fig. S4** SEM images of $CaH_2$-3Zn after 10 cycles using backscattered electrons and corresponding EDS spectrum.

(1) Chiotti, P.; Hecht, R., Thermodynamic Properties of the Calcium-Zinc System. *AIME MET SOC TRANS* 1967, **239**, 536-541.

(2) Itkin, V.; Alcock, C., The Ca-Zn (Calcium-Zinc) System. *Bulletin of Alloy Phase Diagrams* 1990, **11**, 328-333.

(3) Vapor Pressure Calculator. https://www.iap.tuwien.ac.at/www/surface/vapor_pressure (accessed May, 2020)

(4) Hodge, W.; Jaffe, R.; Gonser, B. *Calcium and Calcium-Base Alloys*; BATTELLE MEMORIAL INST COLUMBUS OH: 1949.