The effect of $Sr(OH)_2$ on the hydrogen storage properties of the $Mg(NH_2)_2$ -2LiH system

Hujun Cao,^{a*} Han Wang,^b Claudio Pistidda,^a Chiara Milanese,^c Weijin Zhang,^b Anna-Lisa Chaudhary,^a Antonio Santoru,^a Sebastiano Garroni,^d Jozef Bednarcik,^e Hanns-Peter Liermann,^e Ping Chen,^b Thomas Klassen^a and Martin Dornheim^a

a. Institute of Materials Research, Materials Technology, Helmholtz-Zentrum Geesthacht GmbH, Max-Planck-Straße 1, D-21502 Geesthacht, Germany.

E-Mail: hujun.cao@hzg.de; Fax: +49 04152 / 87-2625; Tel: +49 04152 / 87-2643

- b. Dalian National Laboratory for Clean Energy, Dalian Institute of Chemical Physics,
 Chinese Academy of Sciences, Dalian 116023, China.
- c. Pavia H₂ Lab, Department of Chemistry, Physical Chemistry Section, University of Pavia, Viale Taramelli 16, I-27100 Pavia, Italy
- d. Department of Chemistry and Pharmacy, INSTM, Via Vienna 2, I-07100 Sassari, Italy
- e. Deutsches Elektronen-Synchrotron a Research Centre of the Helmholtz Association, Notkestraße 85, Germany.

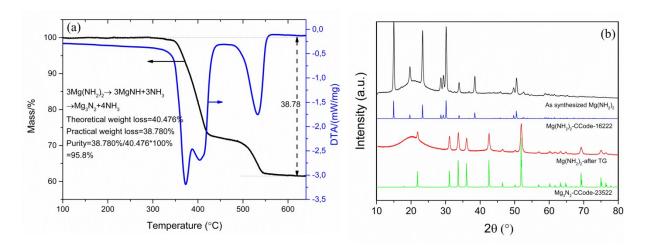


Figure S1. (a) TG-DTA curves of the as prepared $Mg(NH_2)_2$, heated from 30 to 650 °C with a heating rate of 10 °C/min, under 50 ml/min Argon flow. (b) PXD of the as synthesized $Mg(NH_2)_2$ and after TG (Mg_3N_2) . Based on the TG-DTA and PXD results, the purity of $Mg(NH_2)_2$ is ca. 95.8%. PXD tests were carried out with a Bruker D8 discover X-ray diffractometer, using Cu radiation (λ =0.154184 nm, 50 kV, 1000 μ A), with a scanning rate of 0.05 °/s. Air tight sample holders were used (Bruker, Germany) to prevent contamination of the sample.

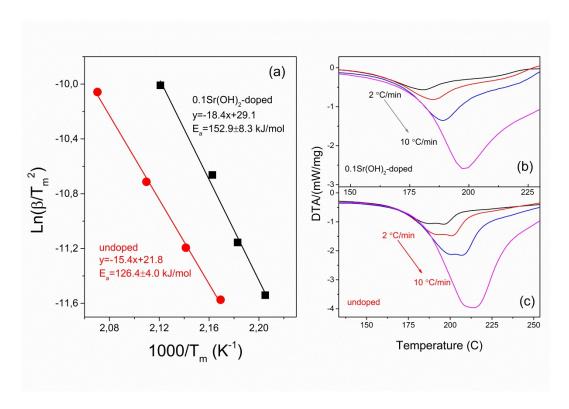


Figure S2. Kissinger plots (a) of the undoped and 0.1Sr(OH)₂-doped samples; and DTA curves of the 0.Sr(OH)₂-doped (b) and the undoped (c) samples with a heating rate of 2, 3, 5 and 10 °C/min, respectively. It should be pointed out that the Ea of the undoped sample was calculated based on the first reaction peak.

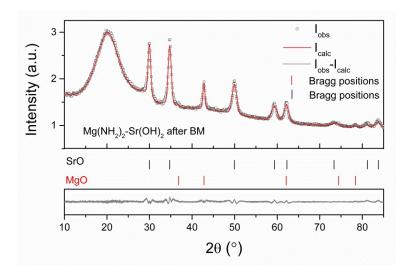


Figure S3. PXD pattern of the ball milled Mg(NH₂)₂-Sr(OH)₂ mixture.

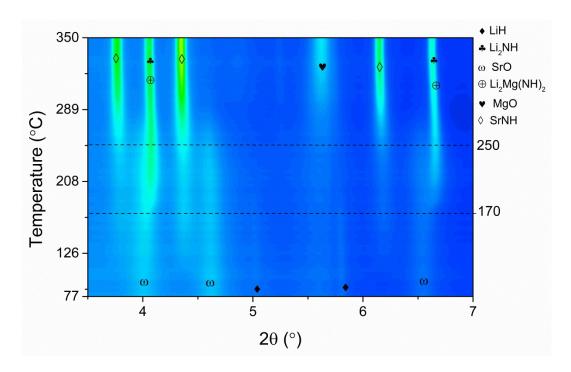


Figure S4.Dehydrogenation contour plot of the 0.2 Sr(OH)₂-doped sample in the 20 range between 3.5 and 7 (°) (heating rate of 10 °C /min, λ =0.20745Å).

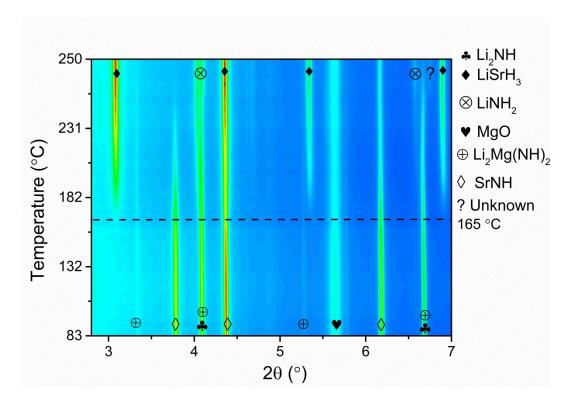


Figure S5. Contour plot of re-hydrogenation curves of $0.2Sr(OH)_2$ -doped sample in the 2θ range between 2.8 and 7 (°) (heating rate of 10 °C /min, λ =0.20745Å).

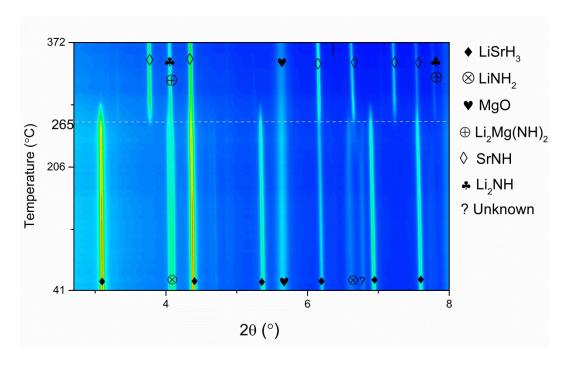


Figure S6. Contour plot of the second dehydrogenation of $0.2Sr(OH)_2$ -doped sample in the 2θ range between 2.8 and 8 (°) (heating rate of 10 °C /min, λ =0.20745Å).