Electronic Supplementary Material (ESI) for Materials Advances. This journal is © The Royal Society of Chemistry 2021

## **Supplementary Information**

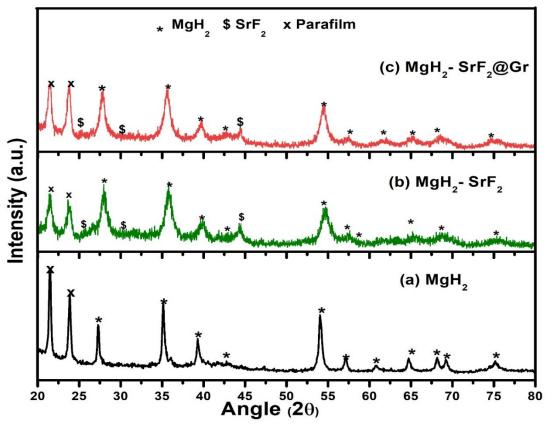
Simultaneous improvement of kinetics and thermodynamics based on SrF<sub>2</sub> and SrF<sub>2</sub>@Gr additives on hydrogen sorption in MgH<sub>2</sub>

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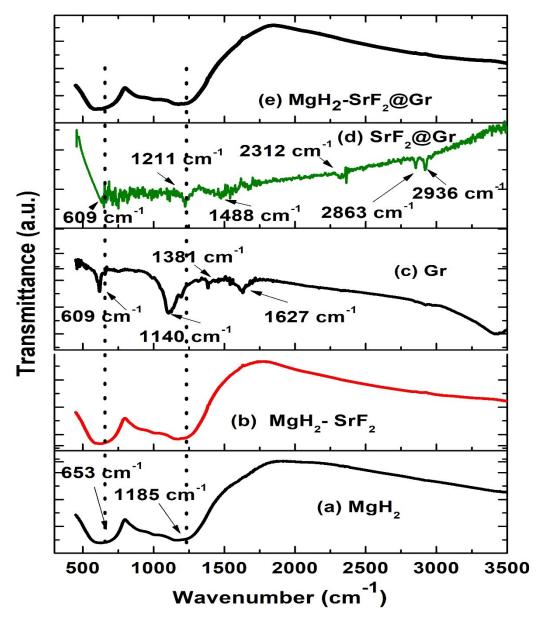
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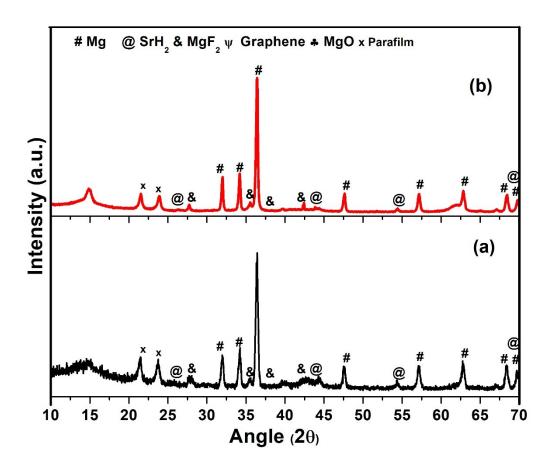
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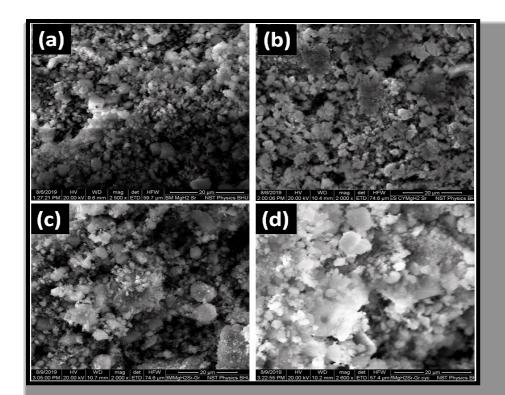
**Figure.S1** XRD of (a) MgH<sub>2</sub> (b) MgH<sub>2</sub>-SrF<sub>2</sub> (c) MgH<sub>2</sub>- SrF<sub>2</sub>@Gr.

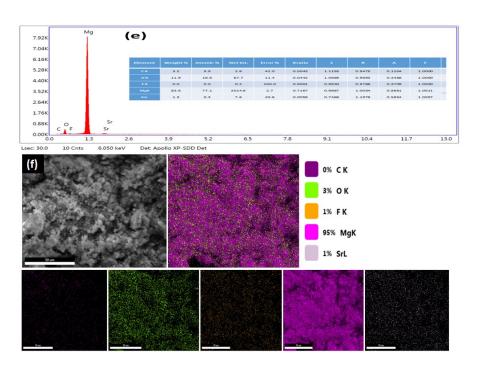


**Figure.S2** FTIR spectra of  $MgH_2$  added (a)  $MgH_2$  (b)  $MgH_2$ -SrF<sub>2</sub> (c) Gr (d) SrF<sub>2</sub>@Gr (e)  $MgH_2$ -SrF<sub>2</sub>@Gr.

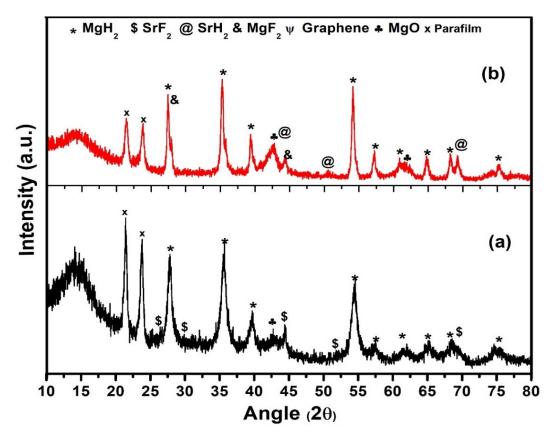


**Figure S3** XRD of (a) Mg-(MgF $_2$ +SrH $_2$ ) (1st dehydrogenation) (b) Mg-SrF $_2$ @Gr (1st dehydrogenation)

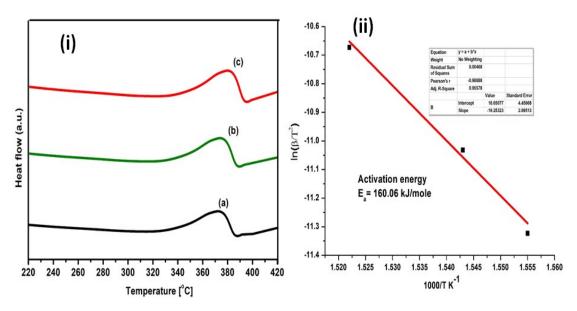




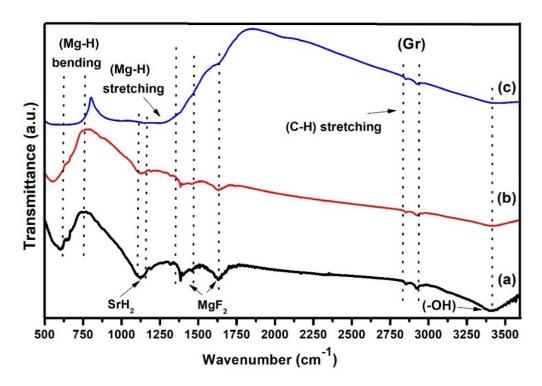
**Figure S4** Scanning electron micrographs of (a)  $MgH_2$ - $SrF_2$  (b) 1 st desorption of  $MgH_2$ - $SrF_2$  ( $Mg-(MgF_2+SrH_2)@Gr)$  (c)  $MgH_2$ - $SrF_2@Gr$  (d) After cycling of  $MgH_2$ - $SrF_2@Gr$  ( $MgH_2$ -( $MgF_2+SrH_2)@Gr)$  (e) EDAX spectra after cycling of  $MgH_2$ -( $MgF_2+SrH_2$ )@Gr sample (f) Elemental mapping after cycling of  $MgH_2$ -( $MgF_2+SrH_2$ )@Gr



 $\textbf{Figure S5} \ XRD \ of (a) \ MgH_2-SrF_2@Gr \ (b) \ After \ 15^{th} \ absorption \ of \ Mg/MgH_2-(MgF_2+SrH_2)@Gr.$ 



**Figure S6** DSC plot of ball milled MgH<sub>2</sub> for 25 hrs at different heating rates (a) 5°C/min (b) 7°C/min (c) 10°C/min (ii) Kissinger plot for the calculation of activation energy.



**Figure S7** FTIR of (a) Mg-(SrH<sub>2</sub>-MgF<sub>2</sub>)@Gr (Ist dehydrogenation) (b) Mg-(SrH<sub>2</sub>-MgF<sub>2</sub>)@Gr (After 14 cycle of dehydrogenation) (c) MgH<sub>2</sub>-(SrH<sub>2</sub>-MgF<sub>2</sub>)@Gr (After 15 cycle of rehydrogenation).