## **Electronic Supplementary Information**

## *In situ* formed ultrafine NbTi nanocrystals from a NbTiC solid-solution MXene for hydrogen storage in MgH<sub>2</sub>

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Fig. S1 TEM and SAED images of NbTiC (a) and NbTiAlC (b).



Fig. S2 Isothermal hydrogenation curves of the milled MgH<sub>2</sub>.



Fig. S3 TPD curves of MgH<sub>2</sub>-9 wt% NbTiC at different heating rates.



Fig. S4 XRD patterns of MgH<sub>2</sub>-*x* wt% NbTiC samples.



Fig. S5 Comparison of dehydrogenation curves of  $MgH_2$  added with 9 wt% and 20 wt% NbTiC.



Fig. S6 XPS spectra of (a) Nd 3d of MgH<sub>2</sub>-Nb<sub>2</sub>C composite and (b) Ti 2p of MgH<sub>2</sub>-Ti<sub>2</sub>C.



Fig. S7 Raman spectra of pristine MgH<sub>2</sub>, NbTiC and MgH<sub>2</sub>-NbTiC composite.