

Supplementary material

Reusable dual functional Mo₂C catalyst for rapid hydrogen evolution via Mg hydrolysis

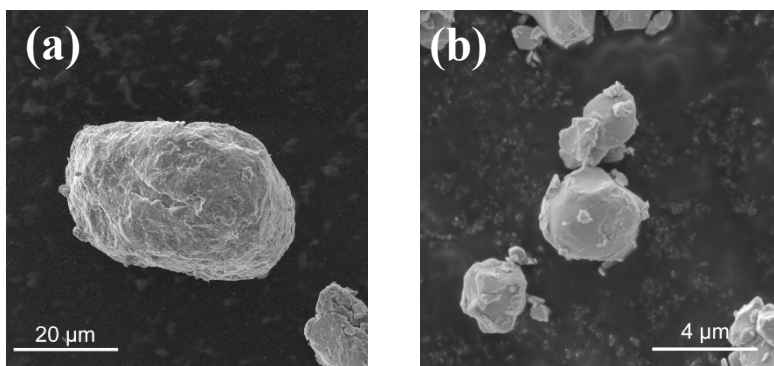


Fig. S1 SEM of raw Mg (a) and raw Mo₂C (b)

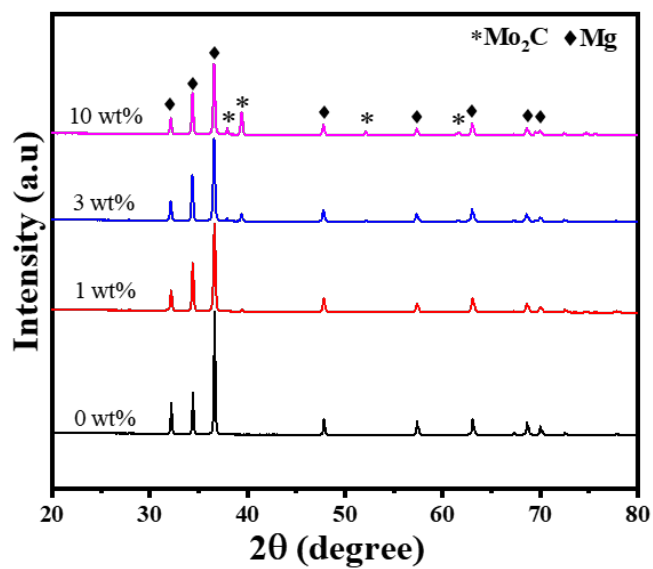


Fig. S2 XRD pattern of ball milled Mg-Mo₂C composite having different Mo₂C contents (0 wt.%, 1 wt.%, 3 wt.% and 10 wt.%)

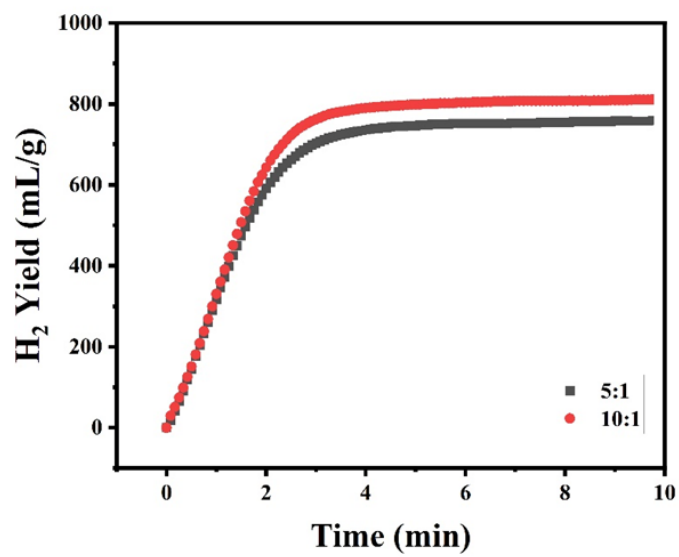


Fig. S3 Hydrogen generation curves of the ball milled Mg-5%Mo₂C composite with ball to powder ratio of 5: 1 and 10: 1.

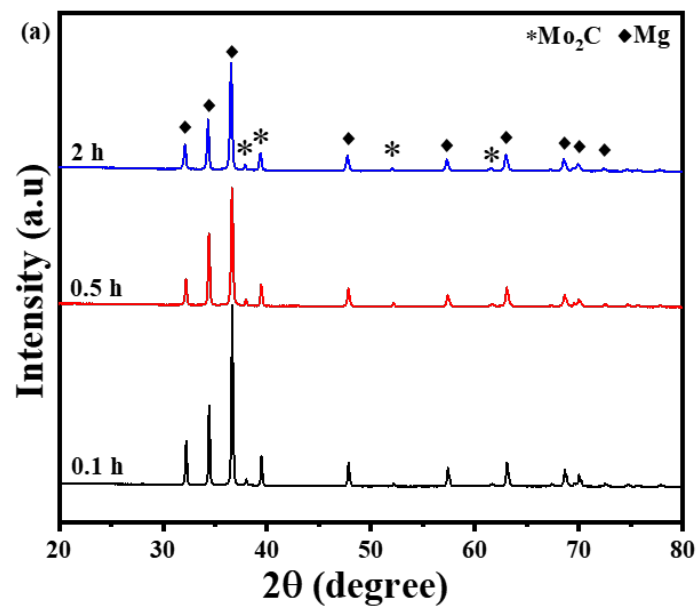


Fig. S4 XRD pattern of ball milled Mg-5%Mo₂C for different milling time (0.1 h, 0.5 h, 2 h)

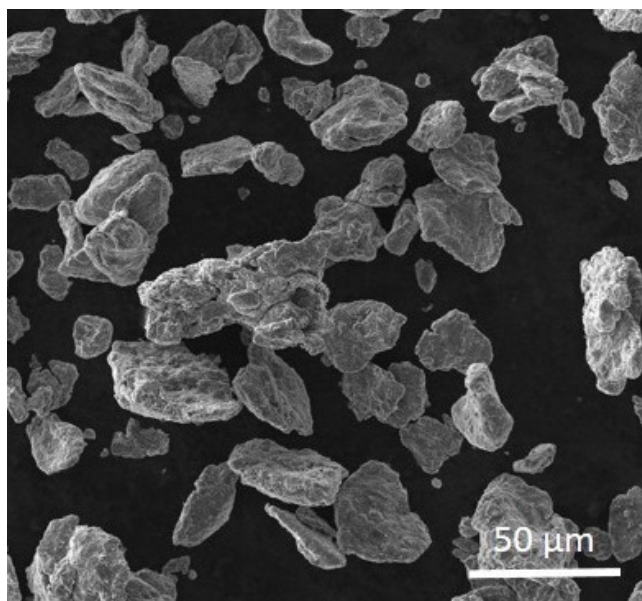


Fig. S5 SEM of ball-milled Mg-Mo₂C composite for 2 h

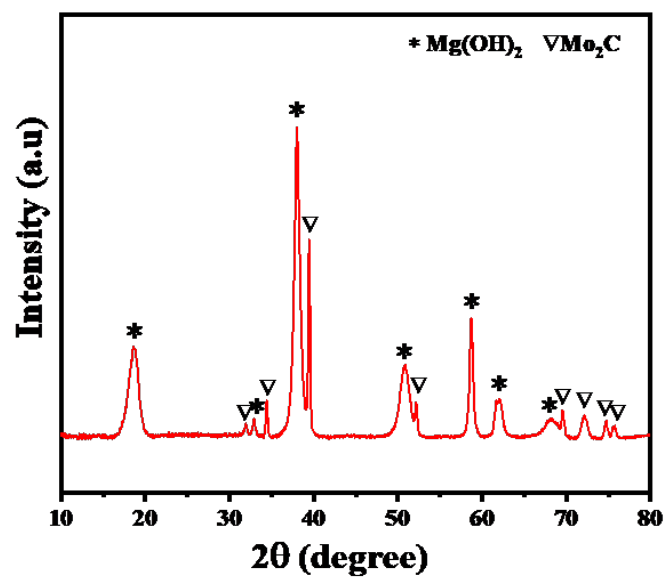


Fig. S6 XRD pattern of hydrolysis by-product of Mg-5%Mo₂C composite with seawater

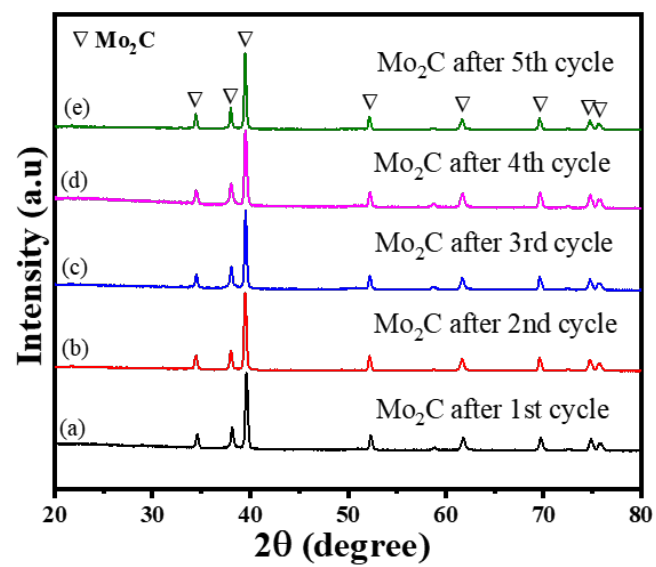


Fig. S7 XRD pattern of Mo₂C after various cycles

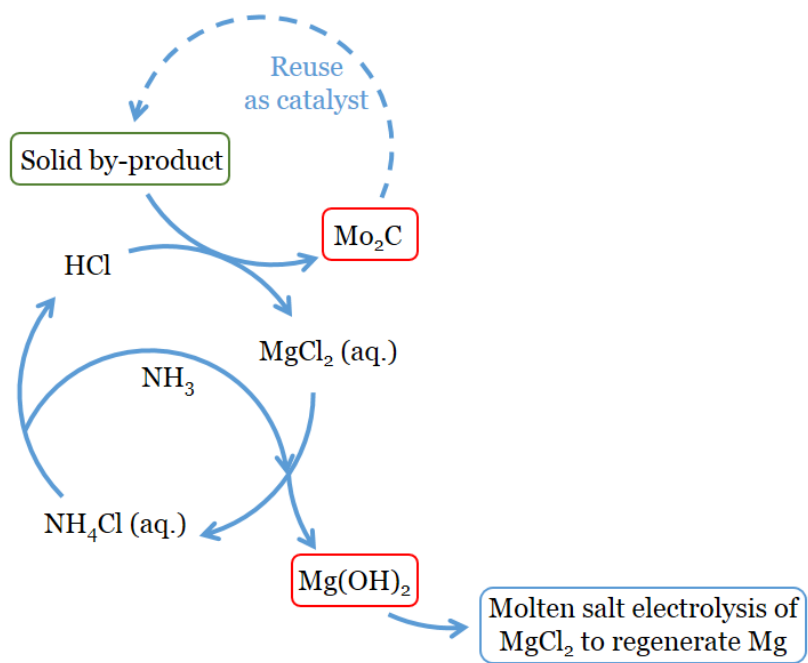


Fig. S8 Recycle pathway of the Mo_2C and $\text{Mg}(\text{OH})_2$

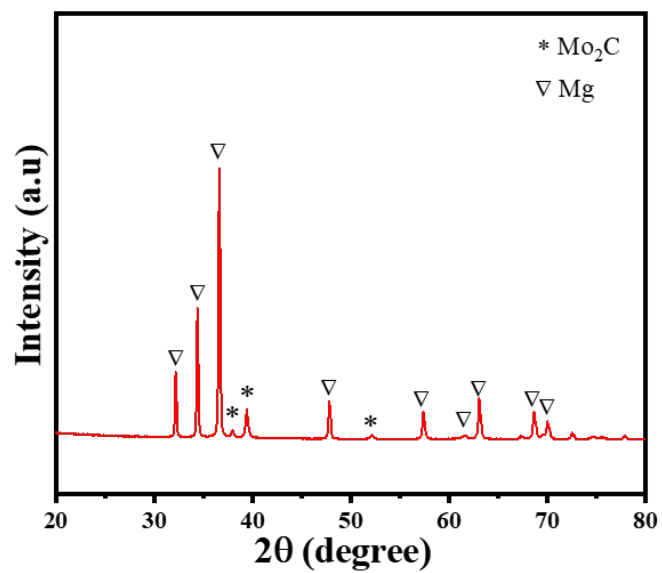


Fig. S9 XRD pattern of hand mixed Mg-5%Mo₂C

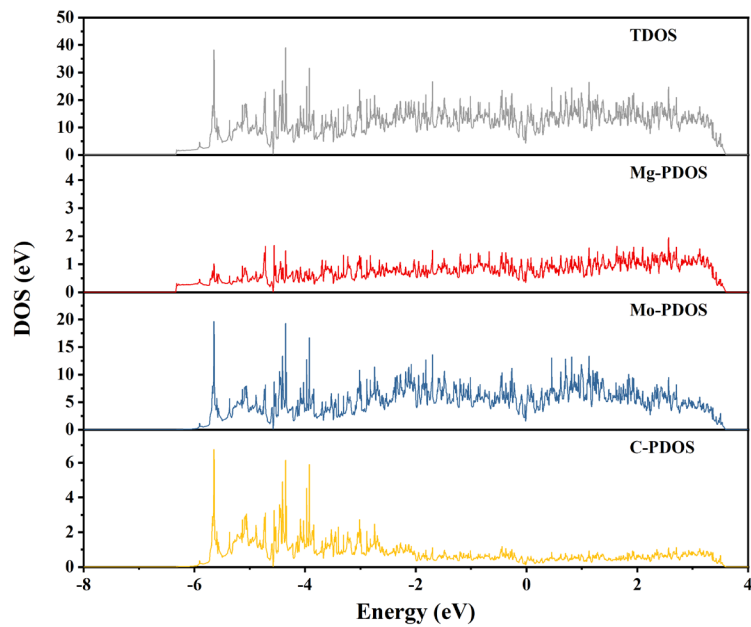


Fig. S10 Density of states calculated for Mg-5%Mo₂C system (the Fermi level is set at 0 eV)

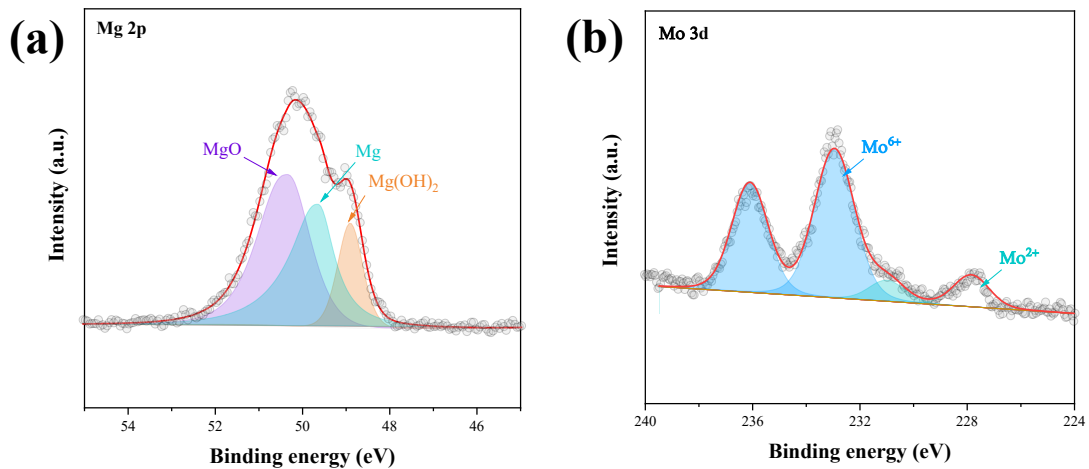
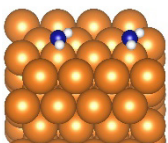
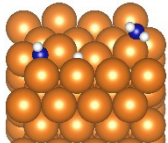
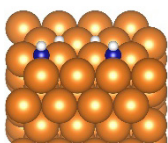
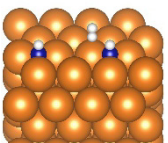


Fig. S11 Mg 2p (a) and Mo 3d (b) XPS spectrum of the hand-mixed Mg-5%Mo₂C

Table S1 The local structure of each step in free energy diagrams

		$2\text{H}_2\text{O}^*$	$\text{H}_2\text{O}^*+\text{OH}^*+\text{H}^*$	$2\text{OH}^*+2\text{H}^*$	$2\text{OH}^*+\text{H}_2 \uparrow$
Mg	Energy (eV)	-0.66	-1.71	-3.57	-2.10
	structure				
Mg+Mo₂C	Energy (eV)	-1.06	-2.60	-4.31	-3.51
	structure	