

# Understanding the Role of Few-layer Graphene Nanosheets In Enhancing the Hydrogen Sorption Kinetics of Magnesium Hydride

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Table S1. Different reaction models consistent with Avrami exponent  $n \approx 1^{1-2}$ .

Model equation	Description
$\alpha = kt$	Surface controlled (chemisorption)
$1 - (2\alpha/3) - (1 - \alpha)^{2/3} = kt$	Contracting volume, 3-d growth diffusion controlled with decreasing interface velocity
$1 - (1 - \alpha)^{1/2} = kt$	Contracting volume, 2-d growth with constant interface velocity
$1 - (1 - \alpha)^{1/3} = kt$	Contracting volume, 3-d growth with constant interface velocity
$-\ln(1 - \alpha) = kt$	Mampel equation (random nucleation approach)

Table S2. Grain size of MgH<sub>2</sub>-5GNS and MgH<sub>2</sub> samples before and after cycling.

Sample	Crystallite size (nm)	
	Before cycling	After cycling
MgH <sub>2</sub> -5GNS	7.3	19.5
MgH <sub>2</sub>	10.8	32

### Notes on calibration and conversion of TPD intensity to weight of hydrogen:

Before the TPD intensity calibrating, the calibration factor is necessary. Generally, the calibration was performed by using a 35.1 mL min<sup>-1</sup> high-purity hydrogen (99.999%) flow rate and 5 °C/min heating rate. The calibration factor can be obtained from the equation as follow:

$$C_f = \frac{A(t)}{I(t)} \times F_{H_2} \quad (1)$$

Where  $C_f$  is the calibration factor,  $A(t)$  is the peak area at time  $t$ ,  $I(t)$  is the peak intensity at time  $t$  and  $F_{H_2}$  is the hydrogen flow rate.

Then the TPD performance of composites were measured by the same flow rate ( $H_2$  was replaced by Ar) and heating rate as the process of calibration. Because there was only  $H_2$  released during the decomposition process, the weight of hydrogen can be calculated from TPD curve by the follow equation:

$$wt\% = \left[ \frac{A_{peak}}{C_f} \times \frac{M_{H_2} PV}{RT} \right] / m \quad (2)$$

Here, wt% is the hydrogen weight,  $A_{peak}$  is the peak area of desorption,  $M_{H_2}$  is molecular of  $H_2$ ,  $P$  is pressure,  $V$  is the volume of six-way valve,  $R$  is the gas constant,  $T$  is the temperature and  $m$  is the weight of the composites.

### References:

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2. Mao, J. F.; Guo, Z. P.; Yu, X. B.; Liu, H. K.; Wu, Z.; Ni, J., Enhanced hydrogen sorption properties of Ni and Co-catalyzed MgH<sub>2</sub>. *Int. J. Hydrogen Energy* **2010**, *35*, 4569-4575.