

# Materials Science and Materials Chemistry

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## Catalytic effect of Ti-based additives on hydrogenation of $MgH_2$

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Various Ti-based additives ( $TiF_4$ ,  $TiO_2$  and  $TiH_2$ ) were added to  $MgH_2$  by ball milling and their catalytic effect on hydrogenation properties was investigated. All these additives significantly improved the dehydrogenation performances of  $MgH_2$  but among them,  $TiF_4$  shows best catalytic effect followed by  $TiO_2$  and  $TiH_2$  sequentially. The activation energy of dehydrogenation was calculated by using Kissinger's equation. The result shows that activation energy decreases from -170.48 kJ/mol for as-milled  $MgH_2$  to -77.58 kJ/mol for  $MgH_2-TiH_2$  and

further lowers to -75.50 kJ/mol to -70.82 kJ/mol for the  $MgH_2-TiO_2$  and  $MgH_2-TiF_4$ . Thermogravimetric analysis (TGA) shows the onset desorption temperature of  $MgH_2$  was also reduced by the addition of different Ti-based additives. XPS studies show that the catalytic effect of these additives on hydrogenation/dehydrogenation kinetics was due to by the formation of different active species.

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