

Accepted Manuscript

Synergistic effects of transition metal halides and activated carbon nanofibers on kinetics and reversibility of MgH_2

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PII: S0022-3697(18)30779-0

DOI: [10.1016/j.jpcs.2018.09.001](https://doi.org/10.1016/j.jpcs.2018.09.001)

Reference: PCS 8714

To appear in: *Journal of Physics and Chemistry of Solids*

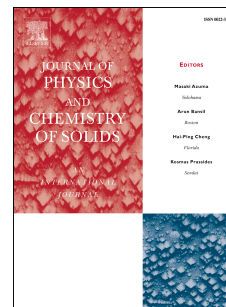
Received Date: 28 March 2018

Revised Date: 30 June 2018

Accepted Date: 3 September 2018

Please cite this article as: P. Plerdsranoy, S. Thiangviriya, P. Dansirima, P. Thongtan, D. Kaewsuwan, N. Chanlek, R. Utke, Synergistic effects of transition metal halides and activated carbon nanofibers on kinetics and reversibility of MgH_2 , *Journal of Physics and Chemistry of Solids* (2018), doi: 10.1016/j.jpcs.2018.09.001.

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1 **Synergistic effects of transition metal halides and activated carbon nanofibers on**
2 **kinetics and reversibility of MgH₂**

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11 MgH₂ doped with transition metal halides (TiF₄, NbF₅, and ZrCl₄) and activated carbon
12 nanofibers (ACNF) for reversible hydrogen storage is prepared by ball milling technique.
13 Transition metal halides provide catalytic effects for de/rehydrogenation kinetics, while
14 ACNF benefits thermal conductivity and hydrogen permeability as well as prevents particle
15 agglomeration during cycling. Significant reduction of onset and main dehydrogenation
16 temperatures of MgH₂ ($\Delta T=243$ and 158 °C, respectively) are achieved by doping with 5-10
17 wt. % of NbF₅, ACNF-TiF₄ and ACNF-NbF₅. During the 1st cycle, the latter samples liberate
18 4.7-5.0 wt. % H₂ within 1 h 30 min, whereas MgH₂ doped with ACNF reaches only 1.5 wt. %
19 H₂. The reaction between MgF₂ and NbH_x ($x<1$) (MgH₂-NbF₅ and MgH₂-ACNF-NbF₅)
20 during dehydrogenation results in the formation of new catalytic active species of Nb-F-Mg
21 favoring kinetics. Upon four hydrogen release and uptake cycles, kinetics and reversibility
22 within 1 h 30 min of MgH₂-ACNF-NbF₅ are preserved at 5.0 wt. % H₂, while those of MgH₂-
23 NbF₅ and MgH₂-ACNF-TiF₄ decay to 4.4 wt. % H₂. Activation energy (E_A) for
24 dehydrogenation of MgH₂ considerably decreases from 140.0 ± 10.2 to 37.8 ± 1.5 kJ/mol after
25 doing with ACNF-NbF₅. Superior performance of MgH₂-ACNF-NbF₅ to MgH₂-NbF₅ is due
26 to synergistic effects of NbF₅ and ACNF. In the case of MH₂-ACNF-TiF₄, the disappearance
27 of active species benefiting kinetic properties and the formation of thermally stable TiH₂
28 account for inferior hydrogen content reversible.

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