

HYDRIDES FOR ENERGY STORAGE

Erika Michela Dematteis,*^a Jussara Barale,^a Marta Corno,^a Paola Rizzi,^a Marcello Baricco^a

^a*Department of Chemistry, Inter-departmental Center Nanostructured Interfaces and Surfaces (NIS), and INSTM, University of Turin, Via Pietro Giuria 7, 10125 Torino, Italy*

e-mail: erikamichela.dematteis@unito.it

Hydrides are investigated for various energy storage applications, including hydrogen storage, solid-state electrolytes, heat storage, etc.[1] With a careful tailoring of composition and a refinement of the microstructure on a nanoscale, properties related to different applications can be significantly improved. In all cases, thermodynamic properties and phase diagrams have to be known in detail.

Hydrides for solid state hydrogen storage and compression have been widely investigated in recent years with the goal to improve hydrogen gravimetric or volumetric density and to match thermodynamic requirements necessary for hydrogen sorption reactions with an equilibrium close to ambient conditions. Results of experimental and theoretical assessments of thermodynamic properties for metal hydrides (based on intermetallic compounds, e.g. TiFe-substituted systems [2,3]) and complex hydrides (e.g. LiBH₄-NaBH₄-KBH₄ system [4–6]) will be reported. The description of thermodynamic properties of the liquid phase in hydrides remains a big challenge, because of lacking experimental data. Examples of assessed phase diagrams will be provided for eutectic mixtures, which may be infiltrated into porous scaffolds to enhance hydrogen sorption properties. Experimental data can vary significantly depending on experimental conditions, because several metastable products can be formed during dehydrogenation reactions.[7] Combining ab-initio calculations and experimental investigations, possible dehydrogenation paths were outlined.

On the basis of hydrogen sorption properties, applications of an optimized solid state hydrogen tanks based on a substituted TiFe material, towards the development of an integrated system at the large scale, will be shown (HyCARE project).[8,9]

References

- [1] Bannenberg, L. J.; Dematteis, E. M.; M.; Baricco, et al. - *Int. J. Hydrogen Energy* **2020**, *45*, 33687–33730.
- [2] Dematteis, E. M.; Cuevas, F.; Latroche, M. - *J. Alloys Compd.* **2021**, *851*, 156075.
- [3] Dematteis, E. M.; Dreistadt, D. M.; Capurso, G.; Jepsen, J.; Cuevas, F.; Latroche, M. - *submitted* **2020**. Pre-print: <https://arxiv.org/abs/2012.00354>
- [4] Dematteis, E. M.; Roedern, E.; Pinatel, E. R.; Corno, M.; Jensen, T. R.; Baricco, M. - *RSC Adv.* **2016**, *6*, 60101–60108.
- [5] Dematteis, E. M.; Pinatel, E. R.; Corno, M.; Jensen, T. R.; Baricco, M. - *Phys. Chem. Chem. Phys.* **2017**, *19*, 25071–25079.
- [6] Dematteis, E. M.; Baricco, M., et al. - *J. Chem. Thermodyn.* **2020**, *143*, 106055.
- [7] Milanese, C.; Dematteis, E. M.; Baricco, M., et al. - *Int. J. Hydrogen Energy* **2019**, *44*, 7860–7874.
- [8] HyCARE focuses on large-scale, solid-state hydrogen storage. *Fuel Cells Bull.* **2019**, *2019*, 11.
- [9] HyCARE project Available online: www.hycare-project.eu.