Design of New Metastable Hydrogen Storage Materials by Binding-Energy Engineering

Kaveh Edalati[1,2,*,#], Ryoko Uehiro[2], Yuji Ikeda[3], Hai-Wen Li[1,4], Hoda Emami[1], Makoto Arita[2], Isao Tanaka[3,5], Etsuo Akiba[1,4,6], Zenji Horita[1,2]

[1]WPI, International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, Fukuoka, Japan
[2]Department of Materials Science and Engineering, Faculty of Engineering, Kyushu University, Fukuoka, Japan
[3]Center for Elements Strategy Initiative for Structure Materials (ESISM), Kyoto University, Sakyo, Kyoto, Japan
[4]International Research Center for Hydrogen Energy, Kyushu University, Fukuoka, Japan
[5]Department of Materials Science and Engineering, Kyoto University, Kyoto, Japan
[6]Department of Mechanical Engineering, Faculty of Engineering, Kyushu University, Fukuoka, Japan

[#]Corresponding author: kaveh.edalati@zaiko6.zaiko.kyushu-u.ac.jp

Mg-based hydrides are considered as potential candiadtes for solid-state hydrogen storage. However, the main drawback of Mg-based hydrides is their high thermodynamic stability, and thus their high dehydrogenation temperature. The objective of this study is to design new Mg-based hydrides with low hydrogen binding energies, which can exhibit reversible hydriding/dehydriding features below 373 K. First-principles calculations using a concept of “binding-energy engineering” were employed to design new compounds and severe plastic deformation using the high-pressure torsion (HPT) method was employed to syntesize the compounds. A few Mg-based metastable phases, which could exhibit reversible hydrogenation/dehydrogenation below 373 K, could be sucessfully fabricated in this study. Details concerning the theoretical desigen and experimental synthesis of these metastable compounds will be discussed in this talk.