

Electronic Supporting Information (ESI)

Entropy differences between hydrides and other elements

Yoshitugu Kojima^{*a} and Masakuni Yamaguchi^b

^a Natural Science Center for Basic Research and Development, Hiroshima University,
1-3-1, Kagamiyama, Higashi-Hiroshima, Hiroshima 739-8530, Japan.

^b Graduate School of Advanced Sciences of Matter, Hiroshima University, 1-3-1,
Kagamiyama, Higashi-Hiroshima, Hiroshima 739-8530, Japan.

* Corresponding author. Tel.: +81 82 424 3904; fax: +81 82 424 5744.

E-mail address: kojimay@hiroshima-u.ac.jp

Table S1 Volume difference, standard entropy difference and standard enthalpy difference.

Hydrides	Volume difference $\Delta V / \text{cm}^3/\text{molH}_2$	Standard entropy difference $\Delta S / \text{J/KmolH}_2$	Standard enthalpy difference $\Delta H / \text{kJ/molH}_2$
LiH	-5.61	-18.3	-181
NaH	-12.9	-22.3	-113
KH	-31.8	-29.3	-115
RbH	-45.2	-39.3	-108
CsH	-63.6	-39.3	-114
MgH ₂	4.18	-1.60	-75.3
CaH ₂	-1.26	-0.30	-182
SrH ₂	-5.70	-25.6	-198
BaH ₂	-4.44	0.50	-177
TiH ₂	2.68	-1.30	-144
ZrH ₂	2.66	-4.30	-169
NbH ₂	2.49	-2.30	-40.0
ThH ₂	4.80	-1.30	-140
UH ₃	6.17	-7.30	-84.8
LaN ₁₅ H ₆ (LaN ₁₅ H _{6.7})	3.99, 4.20	21.7, 22.7	-30.1, -30.8
TiFeH	3.19	24.7	-28.1
NH ₃	10.9, 13.0	23.7	-50.5
MCH	6.92	8.7	-67.5