

Supporting Information

A systematic first principle study of binary metal hydrides

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Ground State Maps of Binary Metal Hydrogen Systems

Legend

Column 1: Li, Na, K, Rb

Column 2: Be, Mg, Ca, Sr

Column 3: Sc, Y

Column 4: Ti, Zr, Hf

Column 5: V, Nb, Ta

Column 6: Cr, Mo

Column 7: Mn, Tc

Column 8: Fe, Ru

Column 9: Co, Rh

Column 10: Ni, Pd, Pt

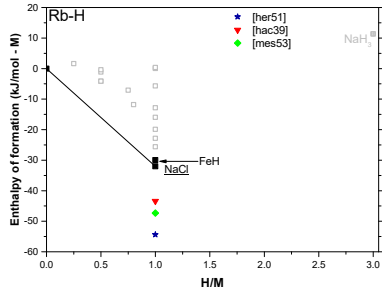
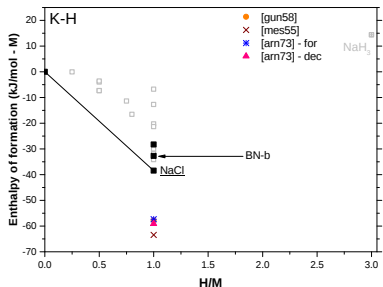
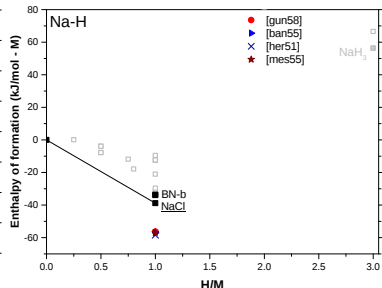
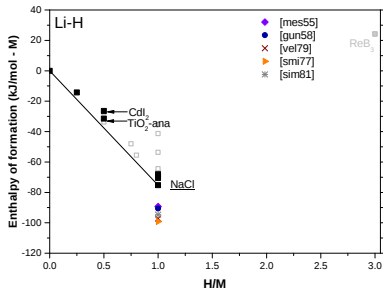
Column 11: Cu, Ag

Column 12: Zn, Cd

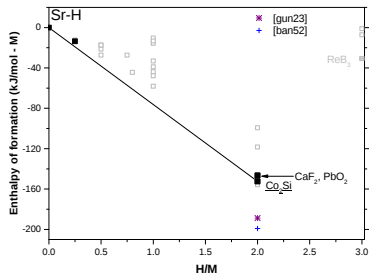
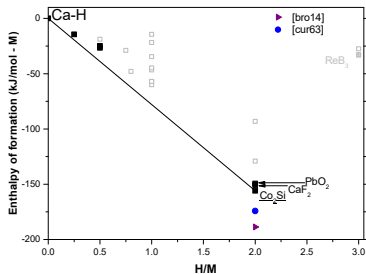
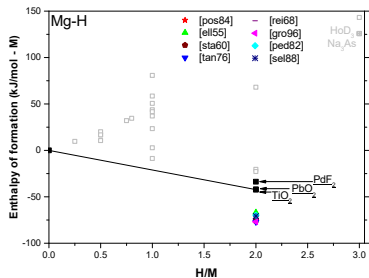
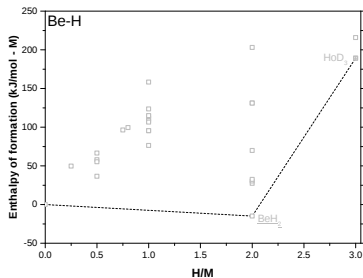
Legend

- Open gray squares: Raw DFT enthalpies of formation $\Delta E_{\text{DFT}}^{MH_y}$ [kJ/mol] (per 1 metal atom)
- Full black squares: DFT enthalpies of formation corrected with the ZPE $\Delta E_{\text{for,cor}}^{MH_y}$ [kJ/mol]
- Crossed out gray squares: Raw DFT enthalpies of formation [kJ/mol] of prototypes presenting negative phonon frequencies
- Colored symbols: Experimental enthalpies of formation [kJ/mol]
- Black line: Ground-state line

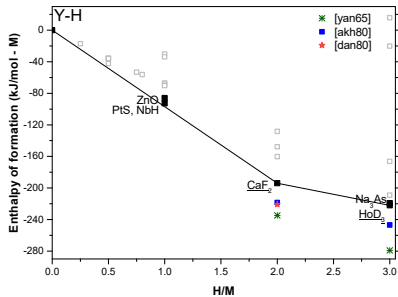
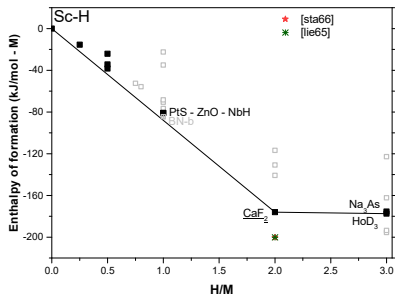
Ground state of Li-H, Na-H, K-H and Rb-H systems



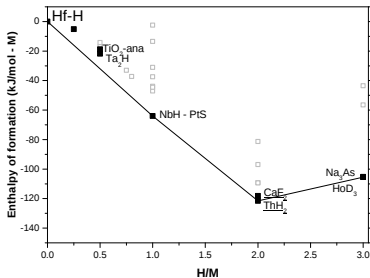
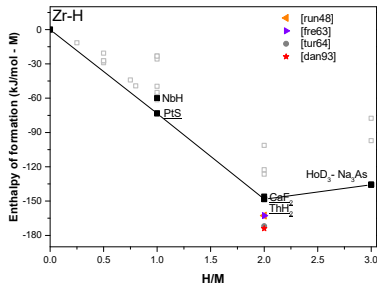
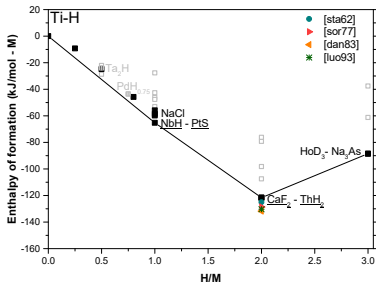
Ground state of Be-H, Mg-H, Ca-H and Sr-H systems



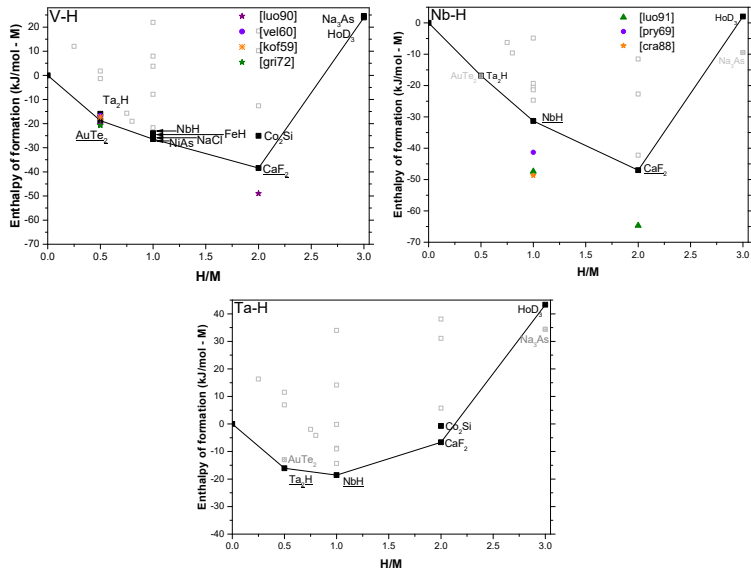
Ground state of Sc-H and Y-H systems



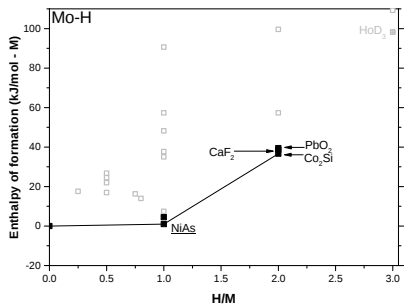
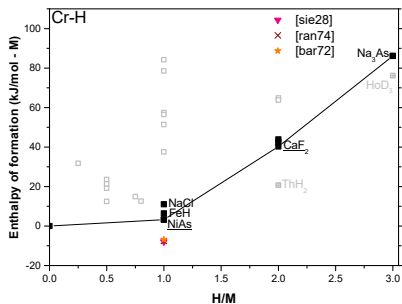
Ground state of Ti-H, Zr-H and Hf-H systems



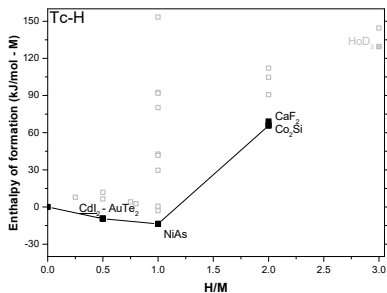
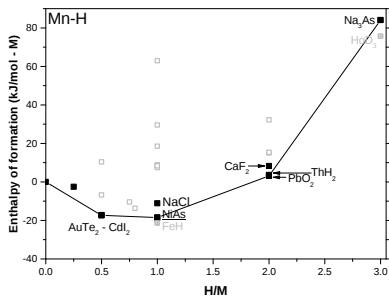
Ground state of V-H, Nb-H and Ta-H systems



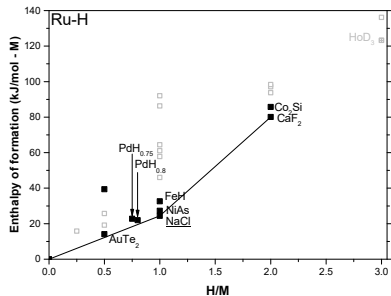
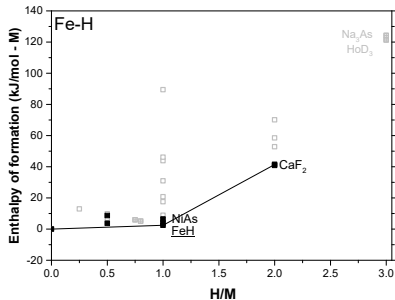
Ground state of Cr-H and Mo-H systems



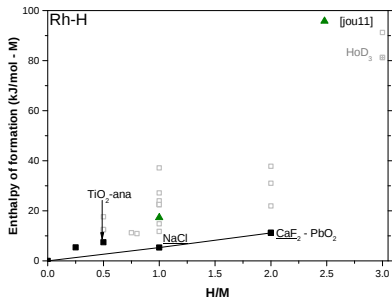
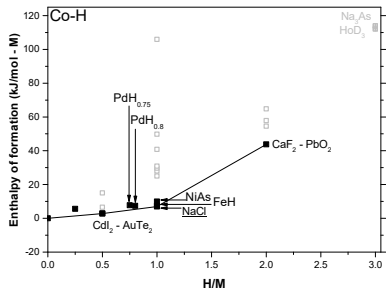
Ground state of Mn-H and Tc-H system



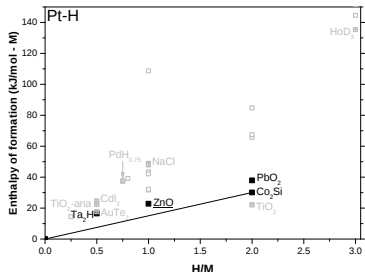
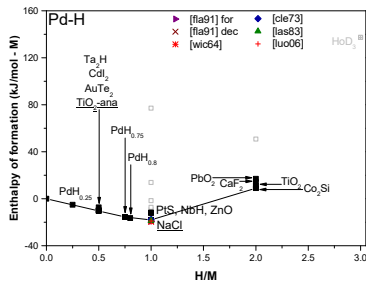
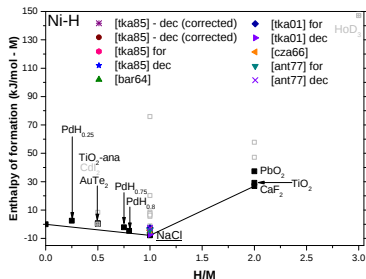
Ground state of Fe-H and Ru-H systems



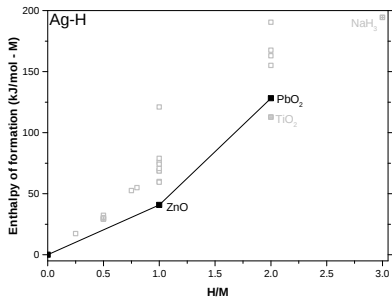
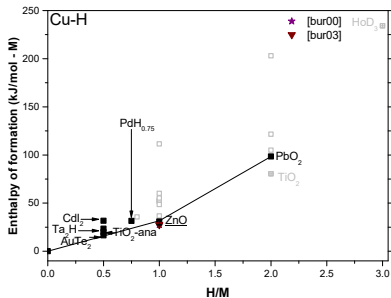
Ground state of Co-H and Rh-H systems



Ground state of Ni-H, Pd-H and Pt-H systems



Ground state of Cu-H and Ag-H systems



Ground state of Zn-H and Cd-H systems

