Homework 10 Advanced Thermodynamics
Due Tuesday November 3, 2020

Rkhis M; Alaoui-Belghiti A; Laasri S; Touhtouh S; Hajjaji A; Hlil EK; Bououdina M; Zaidat K; Obbade S *Enhanced thermodynamic properties of $ZrNiH_3$ by substitution with transition metals (V, Ti ,Fe, Mn and Cr)* Int. J. Hydro. Energy **45** 25002-25012 (2020) investigated substitutional solid solutions for hydrogen storage using transition metals.

a) Rkhis mentions that hydrogen can be stored on materials with high surface area such as carbon nanostructures and zeolites. Explain and give an example of a carbon nanostructure that can be used to store hydrogen and a zeolite for hydrogen storage.
b) Explain the dependence of heat of formation on zeolite structure from the work of Mark E. Davis (Piccione PM; Laberty C; Yang S; Camblor A; Navrotsky A; Davis ME *Thermochemistry of Pure-Silica Zeolites* J. Phys. Chem. B **104** 10001-10011 (2000) and Navrotsky A; Petrovic I; Hu Y; Chen C-Y; Davis ME *Little energetic limitation to microporous and mesoporous materials* Microporous Mat. B 95-98 (1995)).
c) Rkhis is interested in the use of intermetallic hydrides in solid solution with transition metals for reversible hydrogen storage. Define an intermetallic hydride and explain how it can store hydrogen. What is the problem with $ZrNiH_3$ for hydrogen storage?
d) Rkhis has chosen 3d transition metals to substitute for Zr while the literature work has chosen Ti and Nb. Explain the reasoning to choose these transition metals.
e) Figure 3 shows that the gravimetric capacity to store hydrogen increases with increasing content of substituent with the largest increase occurring for titania and the smallest for iron. Explain this increase and the dependence on 3d transition metal substituent.
f) Explain how Figure 4 was obtained.