

**Homework 6**

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```
In [7]: #####  
# Futures  
%matplotlib inline  
# from __future__ import unicode_literals  
# from __future__ import print_function  
  
# Generic/Built-in  
import datetime  
import argparse  
  
# Other Libs  
from IPython.display import display, Image  
#  
from sympy import *  
#  
import matplotlib.pyplot as plt  
plt.rc('xtick', labelsizes=14)  
plt.rc('ytick', labelsizes=14)  
#  
import numpy as np  
np.seterr(divide='ignore', invalid='ignore')  
  
# Owned  
# from nostalgia_util import log_utils  
# from nostalgia_util import settings_util  
__authors__ = ["Osamu Katagiri - A01212611@itesm.mx"]  
__copyright__ = "None"  
__credits__ = ["Marcelo Videia - mvidea@itesm.mx"]  
__license__ = "None"  
__status__ = "Under Work"  
#####
```

## Exercise 1 & 2

```
In [4]: display(Image(filename='./directions/1_2.jpg'))
```

1. Read Chapter 2 of “Chemical Thermodynamics of Materials” of Søren and Grande.
2. Read the paper “Gibbs–Helmholtz equation and entropy” by Ernő Keszei.

- Stolen, S., Grande, T., & Neil L., A. (2004). Chemical Thermodynamics of Materials - Macroscopic and Microscopic Aspects. (J. W. & S. Inc., Ed.). John Wiley & Sons Ltd.
- Keszei, & Erno. (2016). Gibbs – Helmholtz equation and entropy. ChemTexts, 2(15), 15–16.  
<https://doi.org/10.1007/s40828-016-0034-4> (<https://doi.org/10.1007/s40828-016-0034-4>).

## Exercise 3

In [5]: `display(Image(filename='./directions/3.jpg'))`

3. Starting from the Gibbs-Helmholtz equation, demonstrate that the following equation for the standard free energy at a temperature  $T$  can be derived

$$\Delta G^0(T) = \Delta G^0 \frac{T}{T^0} - \Delta H^0 \left(1 - \frac{T}{T^0}\right)$$

- $\frac{G}{T}$  is

$$\left( \frac{\partial \left( \frac{G}{T} \right)}{\partial T} \right)_P = \frac{T \left( \frac{\partial G}{\partial T} \right)_P - G \left( \frac{\partial T}{\partial T} \right)_P}{T^2}$$
$$\left( \frac{\partial \left( \frac{G}{T} \right)}{\partial T} \right)_P = \frac{1}{T} \left( \left( \frac{\partial G}{\partial T} \right)_P - \frac{G}{T} \right)$$

- as  $\frac{\partial G(T,P)}{\partial T} = -S$ , (Gibbs-Helmholtz relation with entropy), then:

$$G = U - TS + PV = H - TS \rightarrow -S = \frac{G - H}{T}$$
$$\left( \frac{\partial \left( \frac{G}{T} \right)}{\partial T} \right)_P = \frac{1}{T} \left( \frac{G - H}{T} - \frac{G}{T} \right)$$

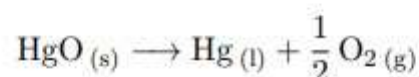
- therefore

$$\left( \frac{\partial \left( \frac{G}{T} \right)}{\partial T} \right)_P = -\frac{H}{T^2}$$

## Exercise 4

In [6]: `display(Image(filename='./directions/4.jpg'))`

4. Determine the temperature at which the following decomposition reaction



becomes spontaneous.

$$\Delta G = \Delta H - T\Delta S$$

$$T = \frac{\Delta H - \Delta G}{\Delta S}$$

$$T = \frac{(-(-90.46) - (-58.43))}{((\frac{1}{2}205.2) + 71.13 - 75.9)}$$

$$T = 1.5219K$$

- let's obtain the equilibrium temperature to ensure  $T$  makes the reaction spontaneous.

$$\Delta G = \Delta H - T\Delta S = 0$$

$$\Delta H - T\Delta S = 0 \rightarrow \Delta H = T\Delta S$$

- divide by  $\Delta S$

$$\frac{\Delta H}{\Delta S} = \frac{T\Delta S}{\Delta S}$$

$$\frac{\Delta H}{\Delta S} = T$$

- calculate  $\Delta S$

$$\Delta S = \sum \Delta S_P - \sum \Delta S_R$$

$$\Delta S = \left( (75.9 + \left( \frac{1}{2}205.2 \right)) - 71.13 \right)$$

$$\Delta S = 178.5 - 71.13$$

$$\Delta S = 107.37 Jmol^{-1}K^{-1}$$

- calculate  $\Delta H$

$$\Delta H = \sum \Delta H_P - \sum \Delta H_R$$

$$\Delta H = \left( \left( 0 + \frac{1}{2} \times 0 \right) - (-90.46) \right)$$

$$\Delta H = 90.46 Jmol^{-1}$$

- substitute  $\Delta S$  and  $\Delta H$

$$T = \frac{\Delta H}{\Delta S}$$

$$T = \frac{90.46 \times 10^3}{107.37}$$

$$T = 842.5K$$

- therefore

At  $842.5K$  the  $\Delta G = 0$  and the system is in equilibrium, therefore the reaction will be spontaneous when  $T < 842.5K$

In [ ]: