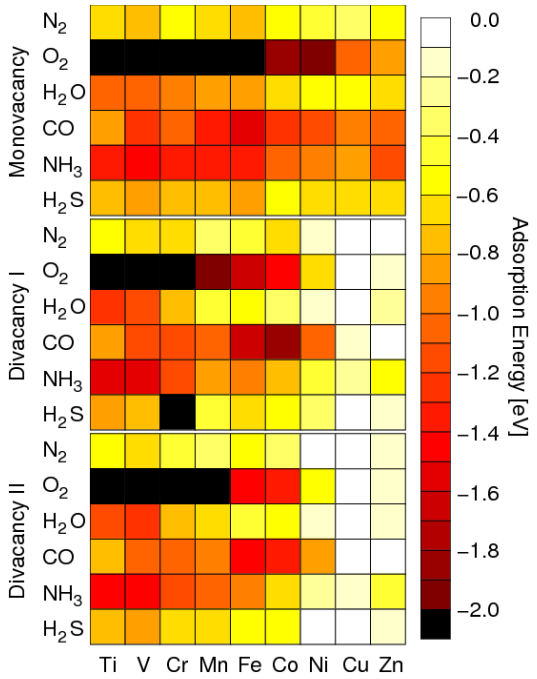
Nanostructural Properties
Optical & Transport Properties of Carbon Nanotubes

Assignment I
Due April 20, 2011[*]

1. You are asked to design a carbon nanotube based chemical sensor for hydrogen sulfide (H_2S), a highly toxic and noxious gas, which becomes poisonous for concentrations between 5–10 ppm, and deadly above 15 ppm. Based on the figure below showing adsorption energies for transition metal doped single-walled carbon nantoubes (TM@SWNTs), which, if any might make suitable detectors for H_2S?



2. Our sensor is supposed to work in air at ground level in a factory in Bilbao, to detect H_2S at night when the area is empty. The the ratio of forward and backward rate constants $K = {}^{k_+}/_{k_-}$ for the adsorption reaction

$$X + * \;\leftrightarrow\; X^*, \tag{1}$$

may be expressed as

$$K[X] \;=\; \exp\left[\frac{-E_{\text{ads}}[X] - TS_{\text{gas}}[X]}{k_B T}\right], \tag{2}$$

where $S_{\text{gas}}[X]$ is the gas phase entropy of species X, k_B is Boltzmann's constant and T is the temperature. Derive an expression the coverage $\Theta[X]$, using the fact that the rate of adsorption r_{ads} is given by

$$r_{\text{ads}} \;=\; k_+\Theta[*]C[X] - k_-\Theta[X] = 0, \tag{3}$$

since we are in equilibrium, where $\Theta[*]$ is the fraction of sites which are unoccupied, $C[X]$ is the gas-phase concentration of species X, and that the sum of all the fractional occupations for all the species in the system is

$$\Theta[*] + \Theta[X] + \sum_{Y\in\mathcal{B}} \Theta[Y] \;=\; 1, \tag{4}$$

where $\mathcal{B}$ is the set of all gas species in the background.

3. Suppose the adsorption energies for the chosen TM@SWNT E_{ads}, concentrations $C[X]$, and gas phases entropies $S_{\text{gas}}[X]$ are as given in Table I. Using the expression derived in the previous question, calculate the coverage of H_2S on the active site at room temperature and H_2 S pressures of 1 ppm and 100 ppm. Note that based on the adsorption energies and concentrations given in Table I, you may argue that the coverage $\Theta[X]$ for some of the gas species listed may be neglected as being negligble.

TABLE I: Equilibrium atmospheric concentrations $C[X]$, gas phase entropies $S_{\text{gas}}[X]$, and adsorption energies $E_{\text{ads}}[X]$, on a TM@CNT, at $T = 300$ K.

X	$C[X]$	$E_{\text{ads}}[X]$	$S_{\text{gas}}[X]$
N_2	74.96%	-0.65 eV	1.988 meV
O_2	20.11%	-2.13 eV	2.128 meV
H_2O	4.00%	-0.79 eV	1.959 meV
CO	96.00 ppb	-1.14 eV	2.050 meV
NH_3	16.32 ppb	-1.07 eV	2.000 meV
H_2S	0.96 ppb	-2.74 eV	2.136 meV

[*] Electronic address: Duncan.Mowbray@gmail.com