Electronic Supplementary Material (ESI) for RSC Advances

SUPPLEMENTARY INFORMATION

Setup for measuring hydrogen sensing capabilities of the ZnO brush beds:Dynamic response of sensitivity of ZnO nano brush beds was measured using a setup which is schematically shown as follows:

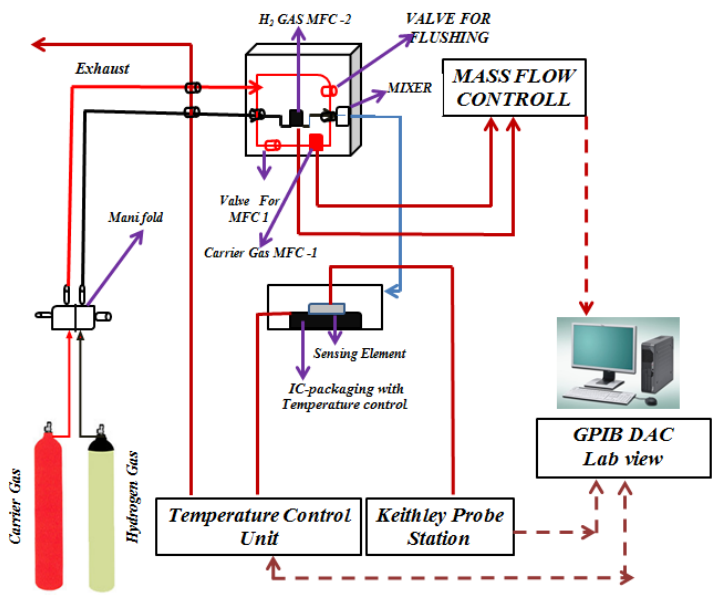

Figure S1 shows schematic of gas sensing set up

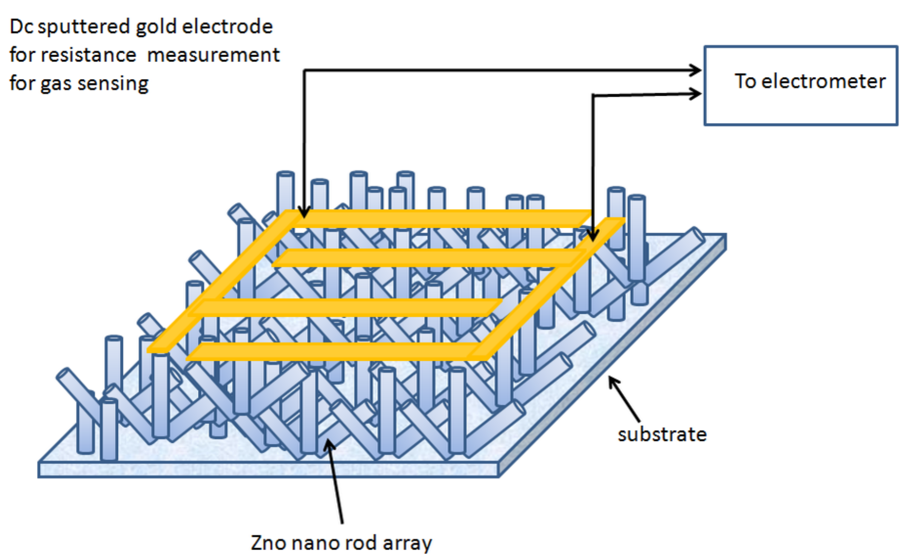

Figure S2: Schematic for electrical connection of ZnO wires with electrodes.

Nanoseed size estimation from the data obtained from UV-Visible spectrophotometer

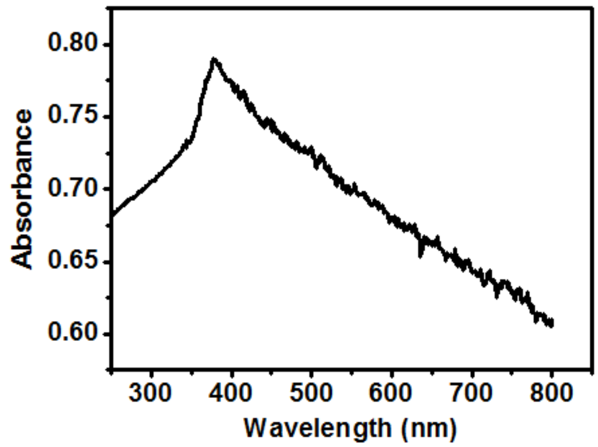

Figure S3 shows the characterization of ZnO seeds by UV-Visible spectroscopy

The particle size can be estimated from the experimental UV-Vis absorption spectrum using the following expression derived from the effective mass model:

$$E_g^* = E_g^{bulk} + \frac{\bar{h}^2\pi^2}{2r^2}\left(\frac{1}{m_e^*}+\frac{1}{m_h^*}\right) - \frac{1.8e^2}{4\pi\varepsilon\varepsilon_0 r} - \frac{0.124e^4}{\bar{h}^2(4\pi\varepsilon\varepsilon_0)^2}\left(\frac{1}{m_e^*}+\frac{1}{m_h^*}\right)^{-1} \quad ..(1)$$

$E_g^* =$ = band gap energy of the nanoparticle, which will be determined from the UV-Visible absorbance spectrum

$E_g^{Bulk} =$ = band gap energy of the bulk ZnO (at room temperature), which has the value of 5.392×(10)^(-19) J

h = Planck's Constant, 6.625×10^{-34} J·s

r = particle radius (m)

m_e = mass of a free electron, 9.11×10^{-31} kg

m_e^* = 0.29 m_e (effective mass of a conduction band electron in ZnO)

m_h^* = 1.21 m_e (effective mass of a valence band hole in ZnO)

e = elementary charge, 1.602×10^{-19} C

$\varepsilon_0 = 8.854\times10^{-12}\,C^2N^{-1}m^{-2}$ (permittivity of free space)

$\varepsilon = 5.7$ (relative permittivity of ZnO)

On putting these values in above equations ,

Using UV- Visible spectra, the cut-off wavelength was determined as $\lambda_c = 379$ nm.

From this value, the band gap of the ZnO was calculated as:

$$E_g{}^* = \frac{(6.626\times10^{-34}\,Js)(3\times10^{8}\,m/s)}{379\times10^{-9}\,m} = 5.24\times10^{-19}\text{ J} = 3.27\text{ eV}$$

Finally, using the band gap, and other known constants, the particle size can be determined from the effective-mass model.

$$E_g{}^* = E_g{}^{bulk} + \frac{\bar{h}^2\pi^2}{2r^2}\left(\frac{1}{m_e{}^*}+\frac{1}{m_h{}^*}\right) - \frac{1.8e^2}{4\pi\varepsilon\varepsilon_0 r} - \frac{0.124e^4}{\bar{h}^2(4\pi\varepsilon\varepsilon_0)^2}\left(\frac{1}{m_e{}^*}+\frac{1}{m_h{}^*}\right)^{-1}$$

where the values of all constants are defined in [1]. This equation can be rearranged to give a quadratic equation as a function of the radius,

$$E_g^{*}r^2 = E_g^{bulk}r^2 + \frac{\bar{h}^2\pi^2}{2}\left(\frac{1}{m_e^{*}} + \frac{1}{m_h^{*}}\right) - \frac{1.8e^2 r}{4\pi\varepsilon\varepsilon_0} - \frac{0.124e^4}{\bar{h}^2(4\pi\varepsilon\varepsilon_0)^2}\left(\frac{1}{m_e^{*}} + \frac{1}{m_h^{*}}\right)^{-1} r^2$$

$$\left[E_g^{*} - E_g^{bulk} + \frac{0.124e^4}{\bar{h}^2(4\pi\varepsilon\varepsilon_0)^2}\left(\frac{1}{m_e^{*}} + \frac{1}{m_h^{*}}\right)^{-1}\right]r^2 + \left[\frac{1.8e^2}{4\pi\varepsilon\varepsilon_0}\right]r - \frac{\bar{h}^2\pi^2}{2}\left(\frac{1}{m_e^{*}} + \frac{1}{m_h^{*}}\right) = 0$$

$$ar^2 + br + c = 0$$

$$r = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

where

$$a = \left[E_g^{*} - E_g^{bulk} + \frac{0.124e^4}{\bar{h}^2(4\pi\varepsilon\varepsilon_0)^2}\left(\frac{1}{m_e^{*}} + \frac{1}{m_h^{*}}\right)^{-1}\right]$$

$$a = 5.232\times10^{-19}J - 5.392\times10^{-19}J + \frac{0.124(1.602\times10^{-19}C)^4}{(6.626\times10^{-34}Js/2\pi)^2(4\pi(5.7)(8.854\times10^{-12}C^2/Nm^2))^2}\bullet$$

$$\left(\frac{1}{0.29(9.11\times10^{-31}kg)} + \frac{1}{1.21(9.11\times10^{-31}kg)}\right)^{-1}$$

$$a = 2.4147\times10^{-20}J$$

$$b = \left[\frac{1.8e^2}{4\pi\varepsilon\varepsilon_0}\right] = \frac{1.8(1.602\times10^{-19}C)^2}{4\pi(5.7)(8.854\times10^{-12}C^2/Nm^2)}$$

$$b = 7.284\times10^{-29}Jm$$

$$c = -\frac{\bar{h}^2\pi^2}{2}\left(\frac{1}{m_e^{*}} + \frac{1}{m_h^{*}}\right) = \frac{-(6.626\times10^{-34}Js/2\pi)^2\pi^2}{2}\bullet\left(\frac{1}{0.29(9.11\times10^{-31}kg)} + \frac{1}{1.21(9.11\times10^{-31}kg)}\right)$$

$$c = -2.5747\times10^{-37}Jm^2$$

$$r = \frac{-7.284\times10^{-29}Jm \pm \sqrt{(7.284\times10^{-29}Jm)^2 - 4(2.4147\times10^{-20}J)(-2.5747\times10^{-37}Jm^2)}}{2(2.4147\times10^{-20}J)}$$

$$r = 4.8nm$$

$$2r = 9.6nm$$

So, the nanoseeds have a particle size of around 9.6 nm, with a band gap of 3.27 eV.