Supporting Information for

Flux improvement, rejection, surface energy and antibacterial study with synthesized TiO_2-Mo.HNTs/PVC nanocomposite ultrafiltration membrane

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2. Experimental Section

Calculation of Porosity and pore size

The pure water flux (J) was calculated using the equation (1) and the rejection of humic acid (HA) and bovine serum albumin (BSA) as model organic foulant were also checked with 100 ppm solution. Foulant solution was fed to the filtration system and after 30 min, reading was noted down for BSA and HA respectively and the rejection percentage was calculated using the below-mentioned equation (2).

$$J = \frac{V}{A \times \Delta t} \ldots\ldots\ldots\ldots\ldots\ldots..(1)$$

where V: the volume collected of pure water, A: the effective membrane area (cm^2), Δt: the permeation time (h).

$$\% R = 1 - \frac{C_P}{C_F} \times 100 \ldots\ldots\ldots(2)$$

where C_P: the concentration of permeation and C_F: the concentration of feed solution, respectively.

The overall membrane porosity (ε) was measured by gravimetric method (Cui et al., 2013) as below mention equation (3)

$$\varepsilon = \frac{\omega_1 - \omega_2}{A \times l \times d_w} \ldots\ldots\ldots\ldots(3)$$

where ω_1; the weight of the wet membrane; ω_2 ; the dry membrane weight, A; the effective membrane area (m^2), d_w :the density of water (0.998 g/cm^3) and l :the membrane thickness (m).

The Guerout-Elford-ferry equation was used for the determination of a mean pore radius (r_m) of the membrane samples using pure water flux and porosity data

$$r_m = \sqrt{\frac{2.9 - 1.7\varepsilon \times 8\eta l Q}{\varepsilon \times \Delta P \times A}} \ldots\ldots\ldots\ldots(4)$$

where g: the viscosity of water (8.9×10^{-4} Pa s), Q: the volume of permeate, pure water per unit time (m^3/s), and ΔP: the operation pressure ($1 kg.cm^{-2}$).

Contact angle measurements

Three liquids (ultrapure water, glycerol and diiodomethane) whose surface tension properties known(Brant and Childress, 2002; Van Oss, 1993), were used for calculating the surface tension elements of membrane surface. Ultrapure water and glycerol are polar in nature, where as diiodomethane is apolar in nature

Table S 1. Surface tension properties of Pure water, glycerol and Diiodomethane liquids at 20°C. [Data taken from van Oss(Van Oss, 1993)]

Liquids	γ^{LW}	γ^{+}	γ^{-}	γ^{AB}	γ_L
	mJ/m^2				
Pure water	21.8	25.5	25.5	51.0	72.8
Glycerol	34.0	3.9	57.4	30.0	64.0
Diiodomethane	50.8	0.0	0.0	0.0	50.8

Calculation of the membrane–liquid interfacial free energy or wetting ability

The contact angle measurement data was not sufficient to explain the wetting ability of the membrane and hence the solid-liquid interfacial free energy was also calculated to ensure surface morphology and surface energy characteristics of the membrane. For the calculation of solid-liquid free energy, a modified Young-Dupre equation (Hurwitz et al., 2010) (5) was used, as follows in equation (5):

$$- \Delta G_{SL} = \left(1 + \frac{Cos\ \theta}{r}\right)\gamma_L \ldots\ldots\ldots\ldots(5)$$

Where the total liquid surface tension: γ_L, the roughness area ratio: r, measured contact angle: θ at room temperature.

Calculating the polar and apolar surface tension elements and interfacial free energy (cohesion or hydrophilicity)

By measuring the contact angle of diidome methane, ultrapure water and glycerol with known surface tension, with the help of an extended Young–Dupré equation (6) the components (LW, AB, γ^{-}, γ^{+}, and γ_L) of the membrane surface tension (Brant and Childress, 2002; Hurwitz et al., 2010) was calculated.

$$\left(1+\frac{Cos\,\theta}{r}\right)\gamma_L = 2\left(\sqrt{\gamma_S^{LW}}\sqrt{\gamma_L^{LW}} + \sqrt{\gamma_S^{+}}\ \sqrt{\gamma_L^{-}} + \sqrt{\gamma_S^{-}}\sqrt{\gamma_L^{+}}\right)\ldots\ldots\ldots(6)$$

where γ^{LW} : Lifshitz-vander waals, γ^{-} electron donor and γ^{+} electron acceptor elements of the membrane surface tension respectively.

The surface tensions were corrected by the surface area ratio in equation (6) and were solved simultaneously using known values of diiodomethane and ultrapure water, glycerol (known surface tension values of γ^{LW}, γ^{+}, and γ^{-}).

The interaction energy per unit area between membrane and liquid, indicate the attraction or repulsion between the two interface when in contact with liquid and this expressed as the free energy of adhesion per unit area (Brant and Childress, 2002; Van Oss, 1993). From the membrane and water elements of the surface tension, the total interfacial free energy by the LW and AB elements of interfacial free energy, was calculated by below-mentioned equation (7a) which often termed as hydrophilicity. Here in the equation if surfaces a and b were of same material (membrane a=b), ΔG_{aca}^{TOT} gives the measurement of interfacial free energy of cohesion.

$$\Delta G_{aca}^{TOT} = \Delta G_{aca}^{LW} + \ \Delta G_{aca}^{AB}\ldots\ldots\ldots\ldots(7a)$$

$$\Delta G_{aca}^{LW} = 2\left(\sqrt{\gamma_c^{LW}} - \sqrt{\gamma_a^{LW}}\right)\left(\sqrt{\gamma_a^{LW}} - \sqrt{\gamma_c^{LW}}\right)\ldots\ldots\ldots\ldots(7b)$$

$$\Delta\ G_{aca}^{AB} = 2\sqrt{\gamma_c^+}\left(\sqrt{\gamma_a^-} + \sqrt{\gamma_a^-} - \sqrt{\gamma_c^-}\right) + 2\sqrt{\gamma_c^-}\left(\sqrt{\gamma_a^+} + \sqrt{\gamma_a^+} - \sqrt{\gamma_c^+}\right) \quad - 2 \ldots\ldots\ldots\ldots(7c)$$

A higher value of free energy is obtained if the membrane is non-cohesive or more hydrophilic when immersed in water.

Antibacterial activity of the membrane

10 ml of LB liquid nutrient medium was taken for inoculation of *E. coli* and the media was shaken (Shaking incubator REMI, India) at 37°C for 24 h. For determining the viable number of cells, the standard serial dilution method was adopted. 0.03 g of membrane sample was cut and then autoclaved (Obromax, India) for sterilization for 20 min. After this membrane samples were immersed in 10 ml solution inoculated by approximately 10^6 colony forming unit (CFU) per ml of *E. coli* culture, for testing the antibacterial property of TiO_2-Mo.HNTs/PVC hybrid membranes. After a period of 1 h of incubation in UV light (Philips 15W UV light), the membrane sample was taken out and washed with saline water. After washing, membrane samples were removed from the washed solution and then the washed solution was diluted with DI water until its concentration came to be 10^{-3} of the initial value.

The dilution solution (0.1 ml) was evenly distributed over the nutrient agar plate after which the test plates were incubated at 37 °C for 24 h. Actual number of colonies present on the plates were calculated by the plate count method. The bacteriostasis rate (BR) was expressed in equation (8) :-

$$BR = \frac{C_0 - C_1}{C_0} \ldots\ldots\ldots\ldots\ldots\ldots(8)$$

where C_0 :the number of colonies grown on the plate treated with control membranes, and C_1 :the number of colonies on the plates treated with hybrid membranes.

3. Result and Discussion

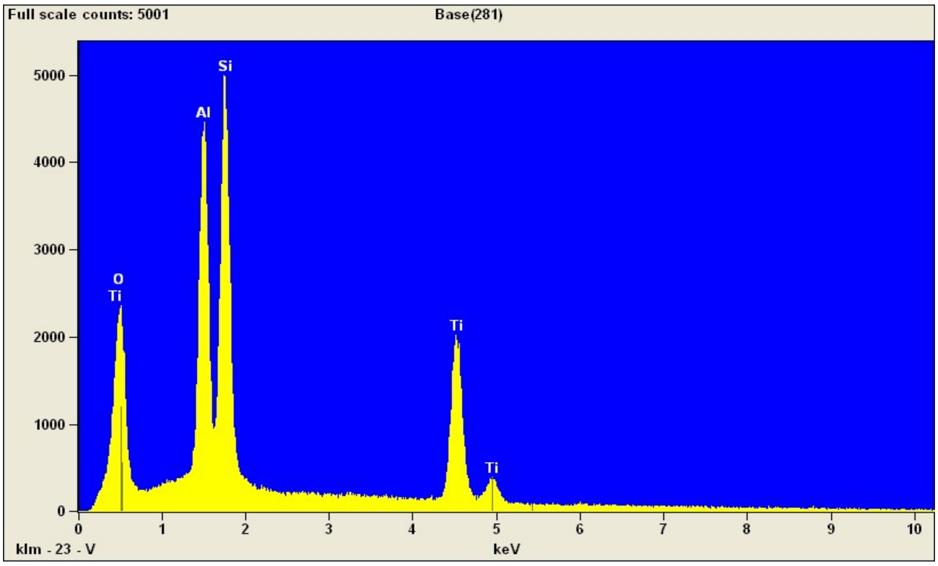

Fig. S 1. EDX spectra of modified TiO_2-Mo.HNTs.

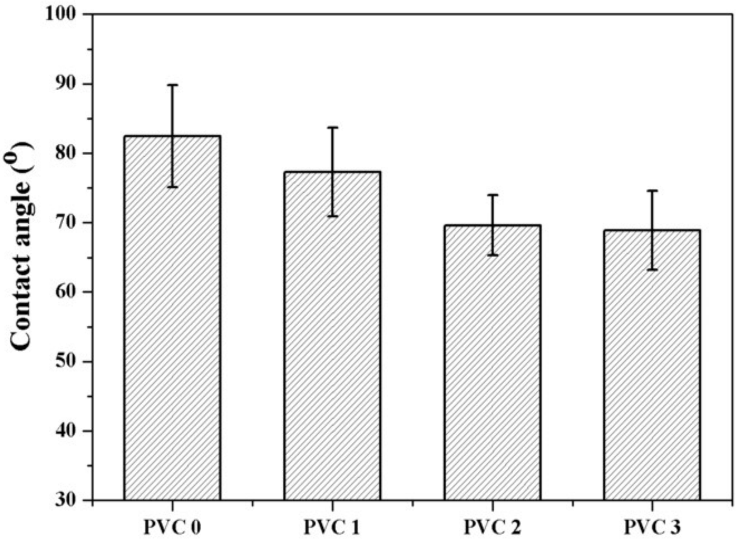

Fig. S 2. Water contact angle measurements of TiO_2-Mo.HNTs (PVC 0- 3wt%) hybrid ultrafiltration membranes.

References

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