Electronic Supplementary Information

Enabling Improved PSF Nanocomposite Membrane for Wastewater Treatment with Selective Nanotubular morphology of PANI/ZnO

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SEM Imaging

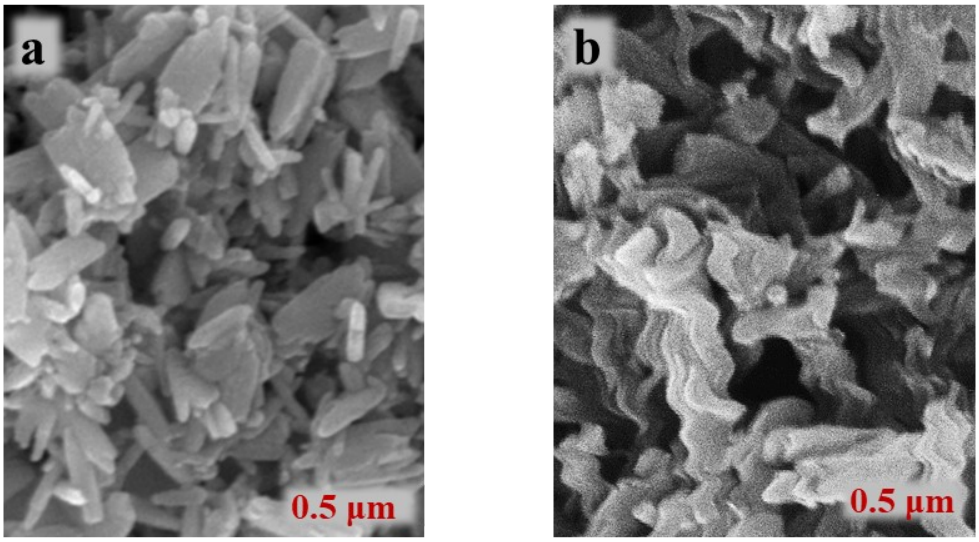

Figure S 1: a) SEM images of ZnO, b) SEM image of PANI.

FTIR Analysis

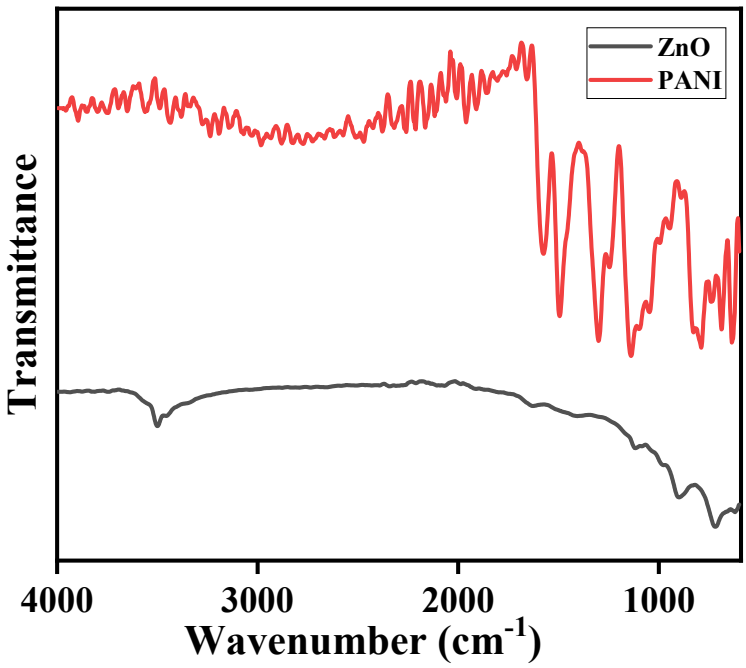

Figure S 2: FTIR spectrum of ZnO and PANI.

The FTIR spectrum of ZnO displayed absorption bands at 454.61 cm^{-1}, 507.44 cm^{-1}, 709.75 cm^{-1}, 896.75 cm^{-1} and 3499.96 cm^{-1}.[1] The band at 3499.96 cm^{-1} is attributed to atmospheric moisture's hydroxyl group, while the bands at 507.44 cm^{-1}, 454.61 cm^{-1} and 896.75 cm^{-1} correspond to the stretching and bending vibrations of the Zn-O bond, indicating the successful formation of ZnO.[2] The aromatic and conjugated structure of PANI was confirmed by obtaining absorptions bands at 3220 cm^{-1} which characterized the N-H stretching vibration of the amine group.[3] The stretching vibrations of C=N and C=C bonds in the quinonoid unit are indicated by an absorption band at 1556 cm^{-1}, while the C=C stretching vibrations and phenylene diamine in the benzenoid unit are represented by a band at 1484 cm^{-1}.[4] Furthermore, the stretching vibration of an aromatic amine (Ar-N) is observed at 1304 cm^{-1}, the stretching vibration of N-Ar-N corresponds to a peak at 1126 cm^{-1}, and the C-H out-of-plane deformation is attributed to a peak at 804 cm^{-1}.[5] The spectrum of pristine PSF exhibited characteristic peaks at 1160, 1256, 1280, 1350 and 1400 cm^{-1}, corresponding to the O=S=O, S-O, C-O-C, S-O symmetric, O-S-O asymmetric and aromatic ring vibrations,[6] respectively.

XRD Analysis

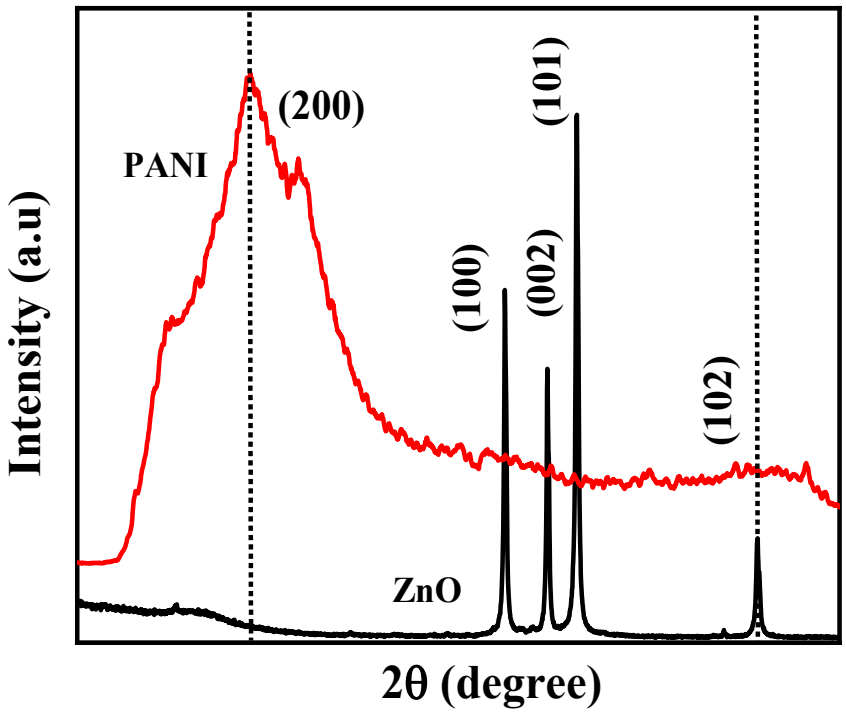

Figure S 3: X-ray Diffractogram of ZnO and PANI.

X-ray diffractogram of ZnO revealed the typical pattern of hexagonal wurtzite ZnO with (100), (002), (101), (102), (110) and (103) diffraction peaks. Crystallite size, obtained by applying Scherrer equation was 22.34 nm. XRD pattern of PANI NT's is showing broad diffraction peaks ranging from 10.1^0 and 30.10^0 due to presence of perpendicular and parallel chains in PANI. [7] The diffraction peaks located at an angle of 2θ= 25.721º and 2θ= 19.311º having d spacing values of 3.461º and 4.593ºA, respectively, showing lower crystallinity or semi-crystalline nature of PANI corresponding to intra-conversion of benzenoid and quinoid units of aromatic rings in polymeric chains. [8, 9]

Table S 1: Optimized Compositions of PSF-PANI Nanocomposite Membranes

Sr. No	Codes	PSF (wt. %)	PANI (wt. %)	DMF (wt. %)
1	PP 0	15	0	85
2	PP 0.05	14.95	0.05	85
3	PP 0.15	14.85	0.15	85
4	PP 0.25	14.75	0.25	85
5	PP 0.30	14.70	0.30	85

Table S2: Composition / codes of pristine and ZnO/(PSF-PANI) Composite membranes.

Membrane	Membrane codes	PSF (wt%)	PANI (wt%)	ZnO (wt%)
Pristine PANI-PSF	PP 0	15	0	0
PSF/PANI/ZnO	PPZ 0.05	14.7	0.25	0.05
PSF/PANI/ZnO	PPZ 0.1	14.65	0.25	0.1
PSF/PANI/ZnO	PPZ 0.15	14.6	0.25	0.15
PSF/PANI/ZnO	PPZ 0.2	14.55	0.25	0.2
PSF/PANI/ZnO	PPZ 0.25	14.5	0.25	0.25
PSF/PANI/ZnO	PPZ 0.3	14.45	0.25	0.3

Strong chemical interaction and intermixing of PANI/ZnO nanofillers in PSF:

In a (PANI/ZnO)-PSF composite membrane, the phrase "strong chemical interaction and intermixing of PANI/ZnO nanofillers in PSF" highlights the significant bonding between

polyaniline (PANI) and zinc oxide (ZnO) nanofillers with the polysulfone (PSF) matrix. This interaction involves hydrogen bonding between PANI's amine groups and ZnO's hydroxyl groups with PSF's sulfone groups, as well as van der Waals forces due to ZnO's slight polarity. [10] Effective intermixing of these nanofillers within the PSF matrix is crucial for optimal membrane performance, ensuring uniform dispersion and preventing agglomeration, which allows for efficient molecular-level interactions with the PSF matrix. [11] In a (PANI/ZnO)-PSF composite membrane, the phrase "strong chemical interaction and intermixing of ZnO/PANI nanofillers in PSF" encompasses several critical aspects. Polyaniline (PANI), a conducting polymer characterized by a backbone of alternating benzene rings and nitrogen atoms, carries positive charges in its doped state. [12] Zinc oxide (ZnO) possesses oxygen-containing functional groups, such as hydroxyl (OH) groups, on its surface. These functional groups facilitate various interactions, including hydrogen bonding, electrostatic interactions, and covalent bonding with other molecules. [13] The intermolecular interactions between PANI and polysulfone (PSF) involve polar-polar interactions. Additionally, PANI and ZnO can establish a network structure within the PSF matrix through π-π stacking, electrostatic attraction, hydrogen bonding, and potential covalent bonding. [14] Collectively, these interactions enhance the mechanical strength and hydrophilicity of the composite material.

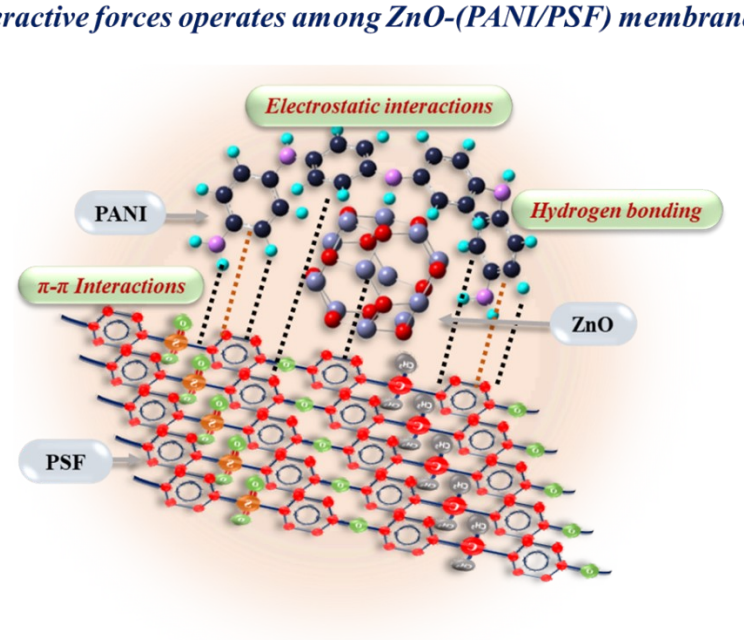

Figure S4: Chemical interactions and intermixing of PANI/ZnO nanofillers in PSF

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