

Supporting Information

Epoxy-Based Vitrimeric Semi-Interpenetrating Network/MXene Nanocomposites for Hydrogen Gas Barrier Application

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Synthesis procedure of MXene ($\text{Ti}_3\text{C}_2\text{T}_x$) from MAX phase (Ti_3AlC_2)

The synthesis of MXene was undergone via the selective etching of Aluminium (Al) from the MAX phase using LiF/HCl. Firstly, LiF powder (4.8 g) was added to HCl (9 M), and the mixture was kept in an oil bath under 30 min of stirring at 35 °C. Next, the MAX phase (3 g) was added gradually while keeping a constant rate of stirring to prevent overheating. The reaction was allowed to proceed at 35 °C for 24 h. After this entire process, the reaction suspension was washed using deionized (DI) water and the precipitate was centrifuged at 7000 rpm for 10 min. This process continued till the pH of the suspension exceeded by 6, assuring the removal of acidic and etched waste with pH neutralization. Furthermore, the final precipitate was redispersed in DI water, purged with nitrogen (N_2) gas for 30 min, and ultrasonicated for 1 h under ice bath conditions. After that, the redispersed solution was centrifuged at 4000 rpm for 20 min, and the supernatant was collected in a glass vial. At last, the delaminated MXene was collected using the vacuum freeze-drying method for the as-prepared supernatant.

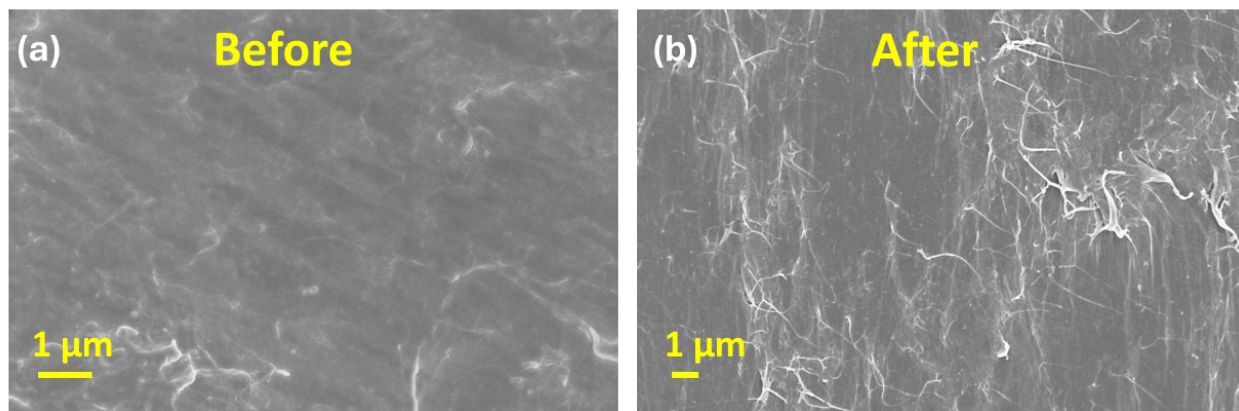


Fig. S1 (a) and (b) FE-SEM images of the EEP film before and after dipping into DMSO, respectively.

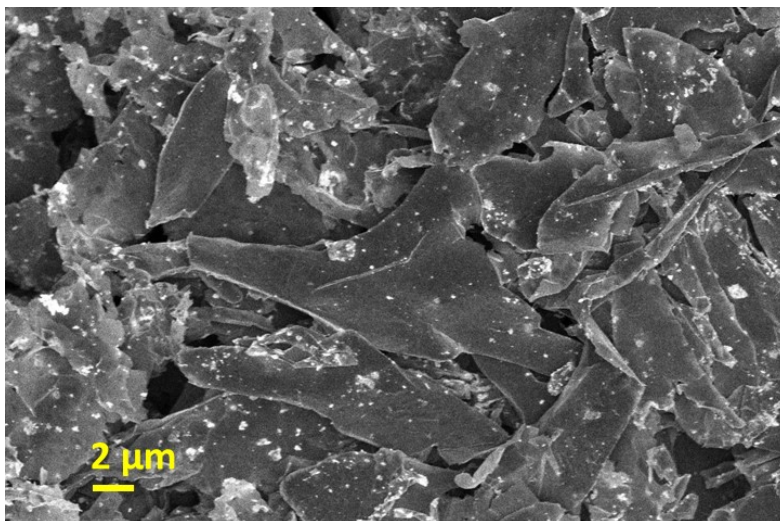


Fig. S2 FESEM scan images of MXene at low magnification showing distribution of flake size.

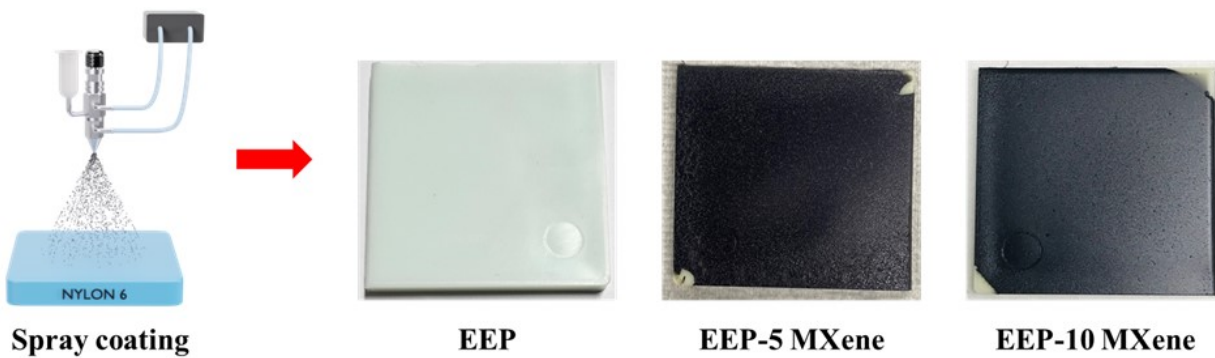


Fig. S3 Representative spray-coated nylon 6 substrates of EEP, EEP-5 MXene, and EEP-10 MXene.

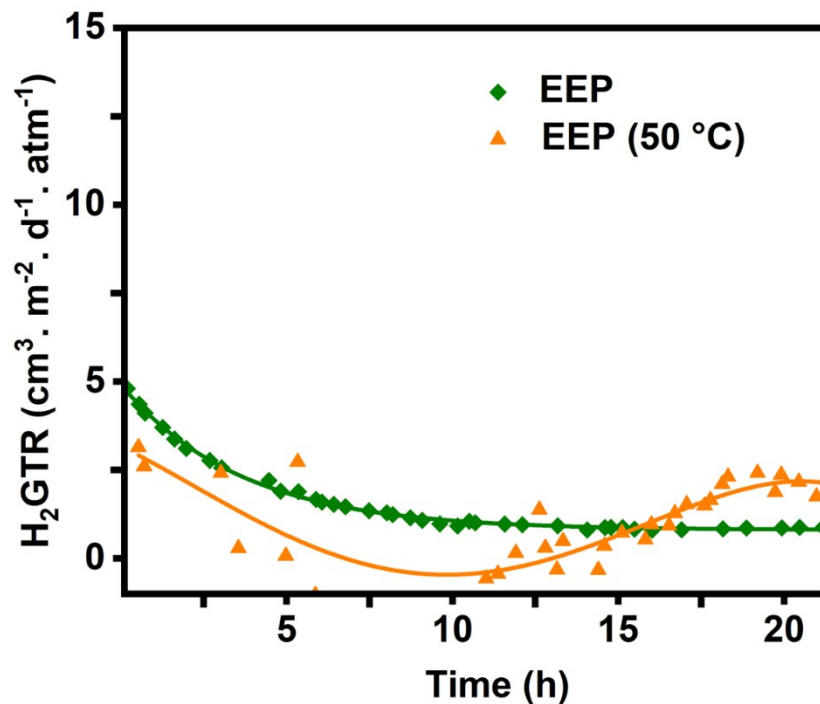


Fig. S4 Compare H₂GTR curves of EEP coated nylon 6 at ambient temperature (RT) and 50 °C.

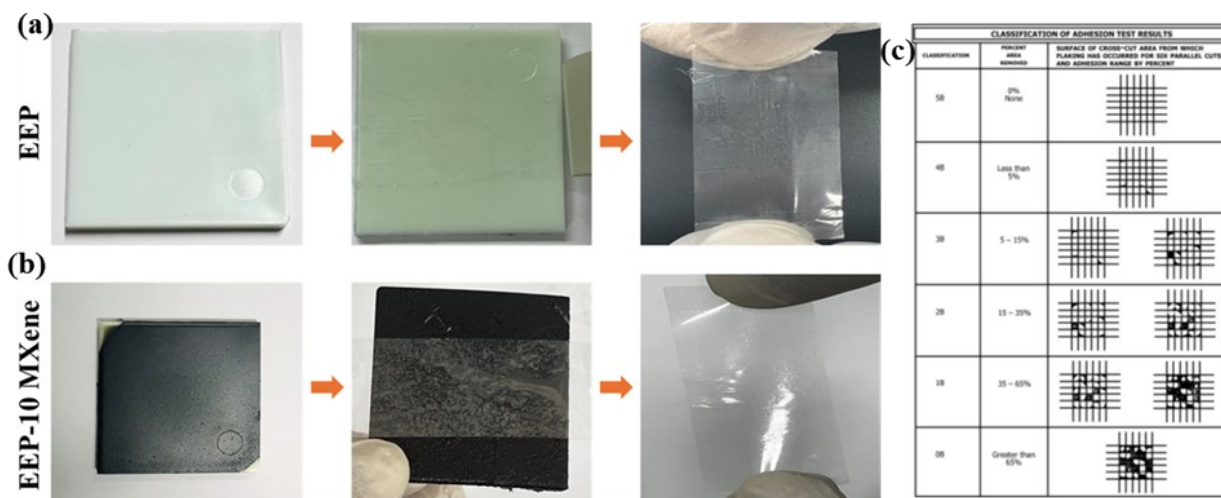


Fig. S5 Analysis of the peel-off adhesion test of coated nylon 6 samples as per ASTM D3359-17, (a) EEP coating; (b) EEP-10 MXene coating; (c) ASTM standard D3359- 17.

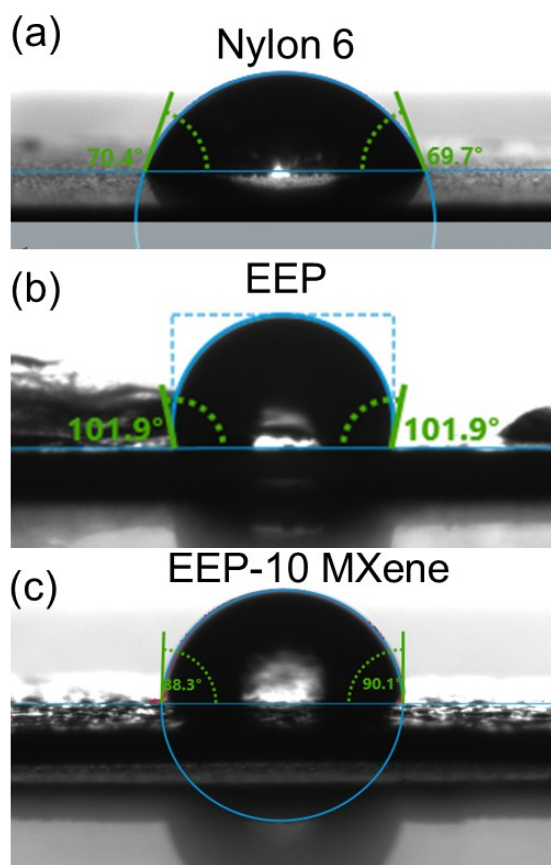


Fig. S6 Water contact angle of (a) uncoated Nylon 6, coated with (b) EEP and (c) EEP-10 MXene at ambient temperature.

Table S1 Atomic wt.% of the constitutive elements in MXene and f-MXene from XPS

Composition	Atomic (%)				
	C1s	Ti2p	O1s	F1s	B1s
MXene	37.69	25.38	16.61	20.32	-
f-MXene	41.51	32.7	24.7	23.29	1.08

Table S2 Comparison of the H₂GTR values obtained from the present work with the previously reported values of 2D filler-based coated polymer nanocomposite films

Films	Filler loading (wt.%)	Substrate	H ₂ GTR ^a	Decrement in H ₂ GTR compared to substrate (%)	P ₁ ^b
HPEI/rGO ¹	16.6	PET/Spray coating	8.0	95	~0.96
Chitosan/PAA/rGO ²	-	PET/Layer-by-layer assembly	102.3	44	-
PVOH/GO ³	80	PET/Spray coating	5	96	0.56
PEI/GO ⁴	-	PET/Layer-by-layer assembly	158.1	41	~0.04
MAPP/mGO-ODA ⁵	60	Nylon/Spray coating	10.6	94	0.26
EVOH/BA/GO ⁶	5	Nylon/Spray coating	6.9	96.1	~0.15
PU/TET-mGO ⁷	22	Nylon/Spray coating	12.8	93	0.15
PU/rGO-HA ⁸	43.3	Nylon/Spray coating	32	82	0.40
f-MXene-GO/EAA ⁹	10	Nylon/Spray coating	2.01	89	0.029
S-IPN2/f-GO-BN ¹⁰	5 and 10	Nylon/Spray coating	0.9 and 0.5	95 and 97	0.01 and 0.006
S-IPN/h-MXene ¹¹	10	Nylon/Spray coating	0.3	98%	0.01
MXene/EEP (Present work)	10	Nylon/Spray coating	0.03	99.8	~0.002

^a Hydrogen gas transmission rate of the coated film (cc·m⁻²·d⁻¹·atm⁻¹).

^b Hydrogen gas permeability coefficient of the coating layer (cc·mm·m⁻²·d⁻¹·atm⁻¹).

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