Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for:

Design and identification of poly(vinyl chloride)/layered double hydroxide@MnO_2 nanocomposite films and evaluation of methyl orange uptake: Linear and non-linear isotherm and kinetic adsorption models

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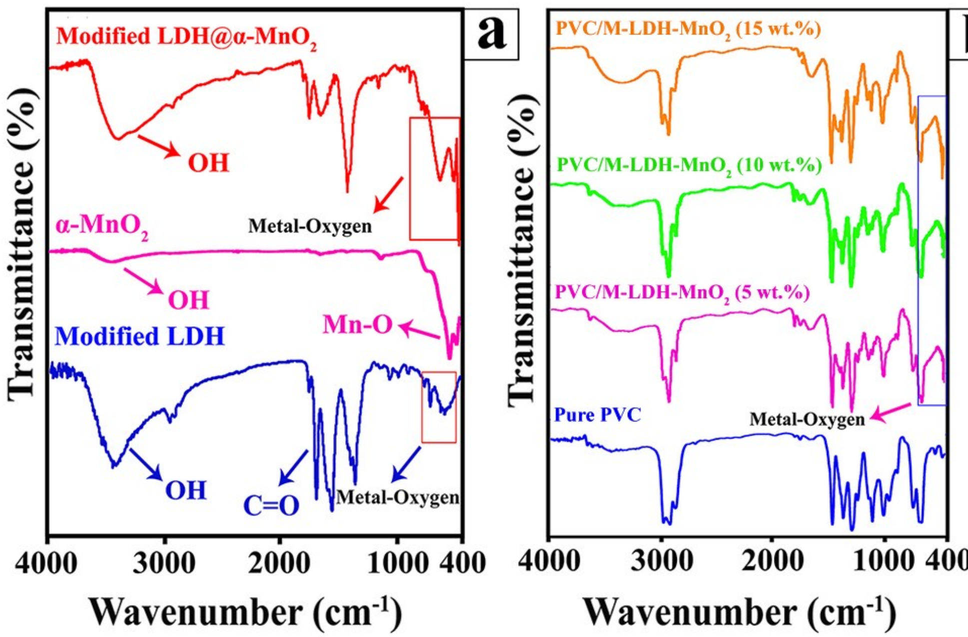

Figure S1 FTIR spectra of the (a) M-LDH, α-MnO_2 nano-rods, and M-LDH@MnO_2 hybrid nano-filler (b) Pure PVC and PVC/M-LDH@MnO_2 nanocomposite films (5, 10, and 15 wt.%).

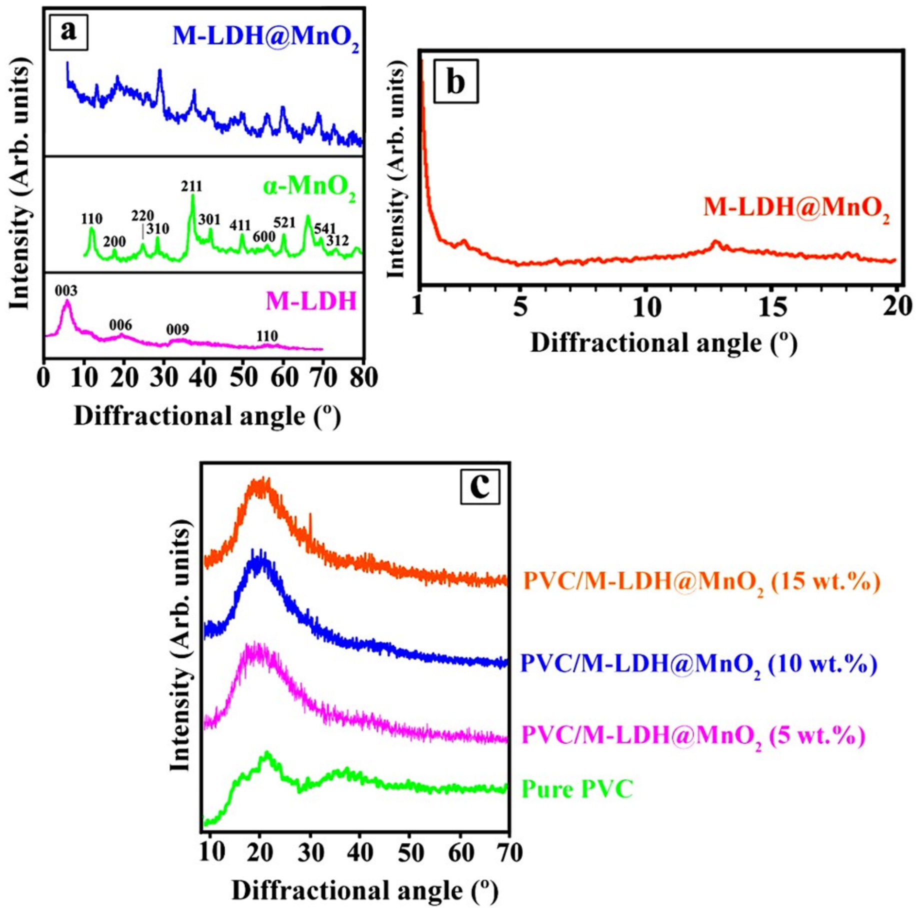

Figure S2 (a) XRD patterns of the M-LDH, α-MnO_2 nano-rods, and M-LDH@MnO_2 hybrid nano-filler, (b) low angle XRD of the M-LDH@MnO_2 hybrid nano-filler, (c) XRD patterns of pure PVC, and PVC/M-LDH@MnO_2 nanocomposite films (5, 10, and 15 wt.%).

Table S1 Atomic percentages from EDX spectra of α-MnO_2 nano-rods, M-LDH, M-LDH@MnO_2 hybrid nano-filler, and PVC/M-LDH@MnO_2 nanocomposite 15 wt.%.

	Atomic percentage							
Sample	K	Mn	Mg	Al	O	N	C	Cl
α-MnO_2 nano-rods	7.2	46.45	-	-	46.35	-	-	-
M-LDH	-	-	5.70	3.26	52.44	15.87	22.73	-
M-LDH@MnO_2 hybrid nano-filler	1.17	6.51	3.73	1.88	56.05	7.56	23.1	-
PVC/M-LDH@MnO_2 nanocomposite 15 wt.%	-	0.55	0.50	0.22	5.04	3.89	65.33	24.27

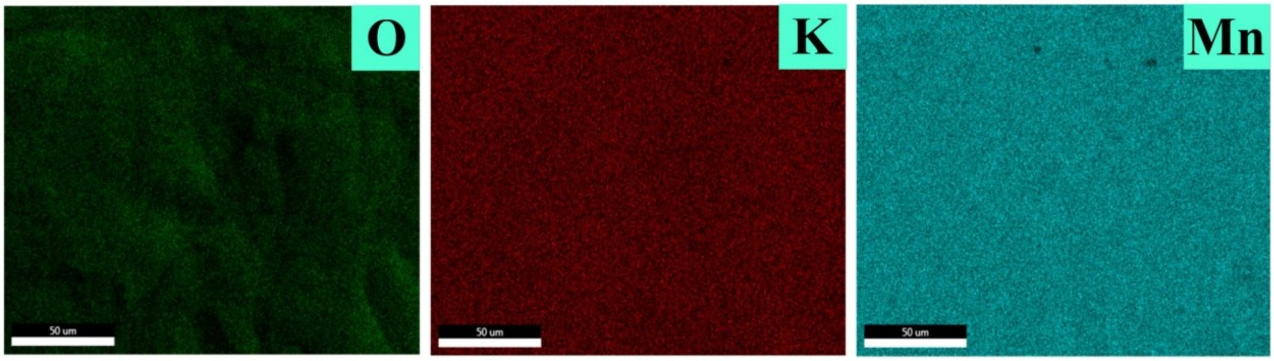

Figure S3 Mapping of α-MnO_2 nano-rods.

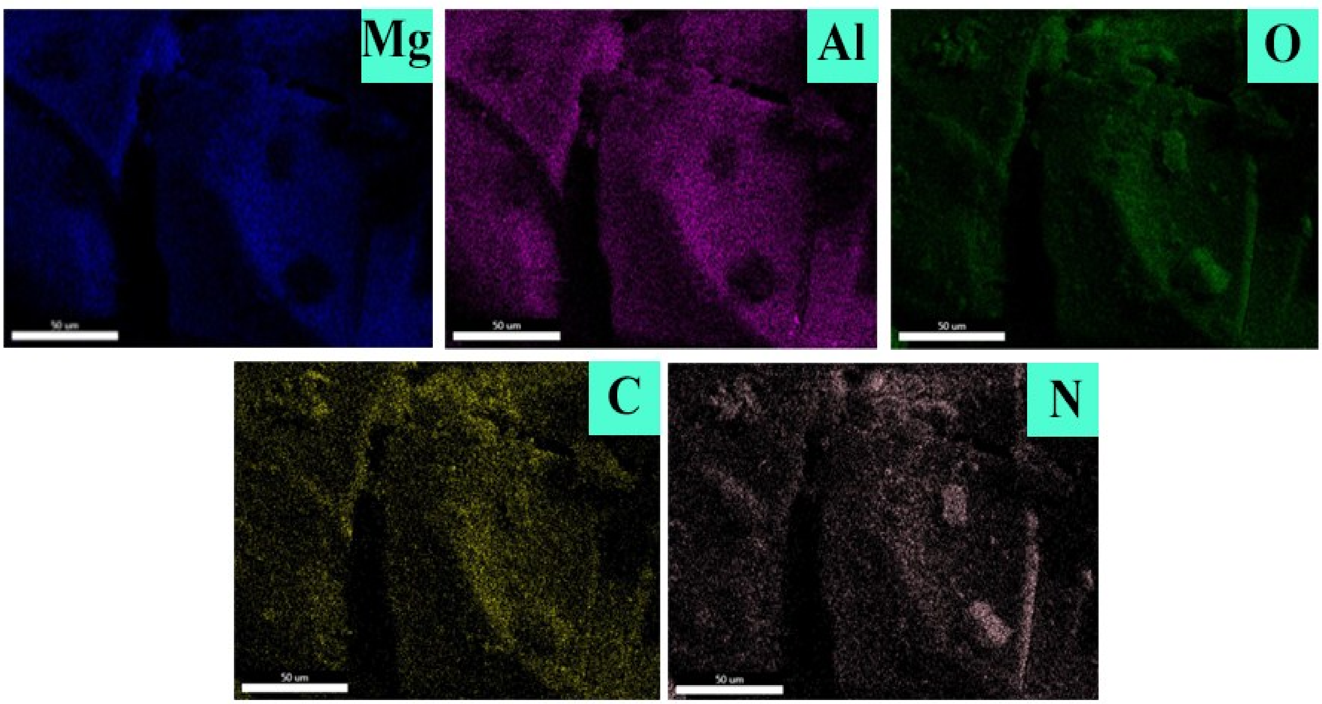

Figure S4 Mapping of M-LDH.

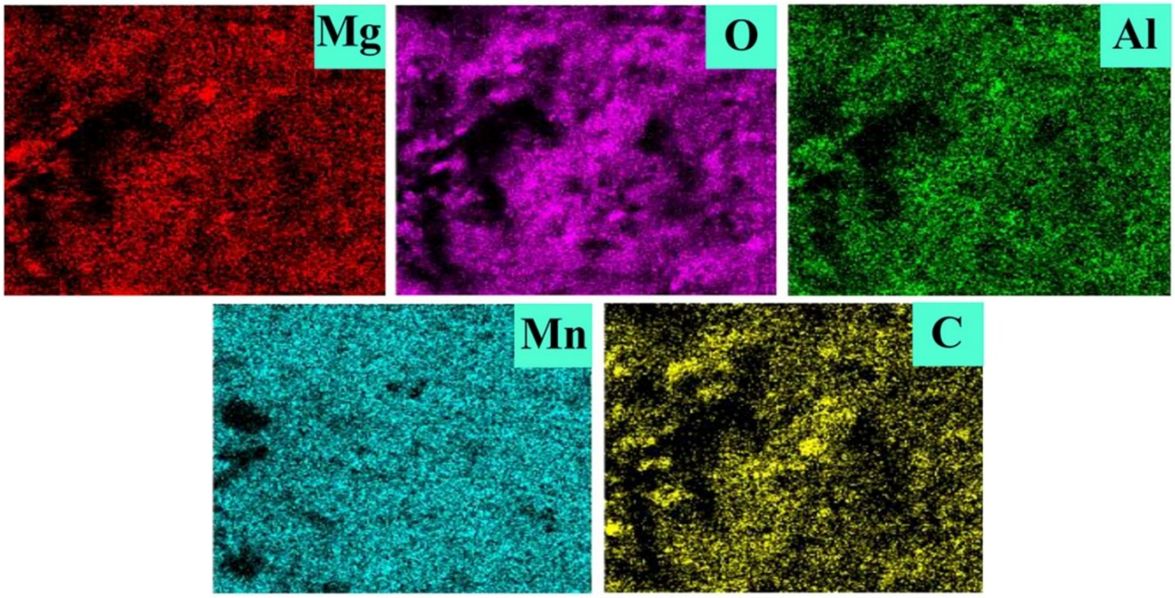

Figure S5 Mapping of M-LDH@MnO_2 hybrid nano-filler.

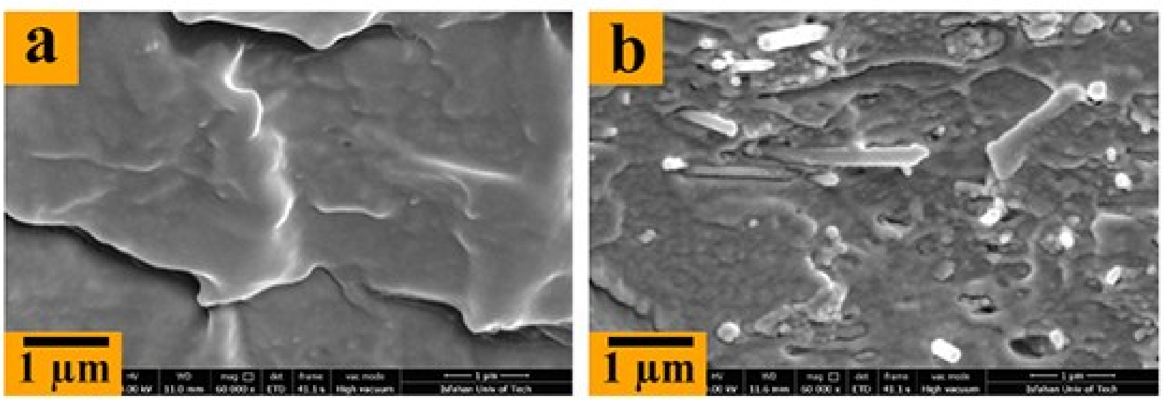

Figure S6 Cross-sectional FESEM images of the (a) PVC and (b) PVC/M-LDH@MnO_2 nanocomposite 10 wt.%.

Table S2 Pore structural information for the M-LDH, M-LDH@MnO_2 hybrid nano-filler, and PVC/M-LDH@MnO_2 nanocomposite 15 wt.%.

Sample	Mean pore diameter (nm)	Total pore volume (cm^3/g)	Reference
M-LDH	38.86	0.007	1
M-LDH@MnO_2 hybrid nano-filler	32.35	0.222	This work
PVC/M-LDH@MnO_2 nanocomposite 15 wt.%	34.95	0.224	This work

Table S3 Char yield values for the α-MnO_2 nano-rods, M-LDH, and M-LDH@MnO_2 hybrid nano-filler.

Sample	Char yield (%)[a]	Reference
α-MnO_2 nano-rods	92	2
M-LDH	44	1
M-LDH@MnO_2 hybrid nano-filler	59	This work

[a] Weight (%) of undecomposed sample after heating at 800 ˚C.

Table S4 Equations for the isotherm, kinetic, Intraparticle, and liquid film diffusion models.

Model	Linear
Langmuir (linear form)	$C_e/Q_e = 1/(Q_m K_L) + C_e/Q_m$
Langmuir (non-linear form)	$Q_e = (Q_m \times C_e \times K_L)/(1 + C_e K_L)$
Freundlich (linear form)	$\ln Q_e = \ln K_F + 1/n \ln C_e$
Freundlich (non-linear form)	$Q_e = K_F \times C_e^{1/n}$
Pseudo-first order (linear form)	$\ln (Q_e - Q_t) = \ln Q_e - k_1 t$
Pseudo-first order (non-linear form)	$Q_t = Q_e[1 - \exp(-k_1 t)]$
Pseudo-second order (linear form)	$t/Q_t = 1/k_2 Q_e^2 + t/Q_e$
Pseudo-second order (non-linear form)	$Q_t = Q_e^2 k_2 t/(1 + Q_e k_2 t)$
Weber's intraparticle diffusion	$Q_t = k_{iP} t^{0.5} + C$
Liquid film diffusion	$\ln (1-F) = k_{fd} . t$

Table S5 r^2 and errors' mathematical equations.

Parameters	Relationships
r^2	$\frac{\sum_{i=1}^{n}(y_{,exp}-\bar{y}_{,cal})^2}{\sum_{i=1}^{n}(y_{,exp}-\bar{y}_{,cal})^2+\sum_{i=1}^{n}(y_{,exp}-y_{,cal})^2}$
RMSE	$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_{,exp}-y_{,cal})^2}$
χ^2	$\sum_{i=1}^{n}\frac{(y_{,\ exp}-y_{,cal})^2}{y_{,cal}}$
SSE	$\sum_{i=1}^{n}(y_{,exp}-y_{,cal})^2$

References

1. S. Mallakpour and M. Hatami, *Appl. Clay Sci.*, 2017, **149**, 28-40.
2. S. Mallakpour, A. Abdolmaleki and H. Tabebordbar, *Europ. Polym. J.,* 2016, **78**, 141-152.