PAR-intercalated Mg/Al layered double hydroxide for efficient adsorption of Acid Fuchsin: experimental study and molecular docking insights

Sara E Abdel Hameed[1], Weam M. Abou El-Maaty[1], Esam A. Gomaa[1], Fathi S. Awad[1, *]

Chemistry Department Faculty of Science, Mansoura University, Mansoura, Egypt

Supporting Information

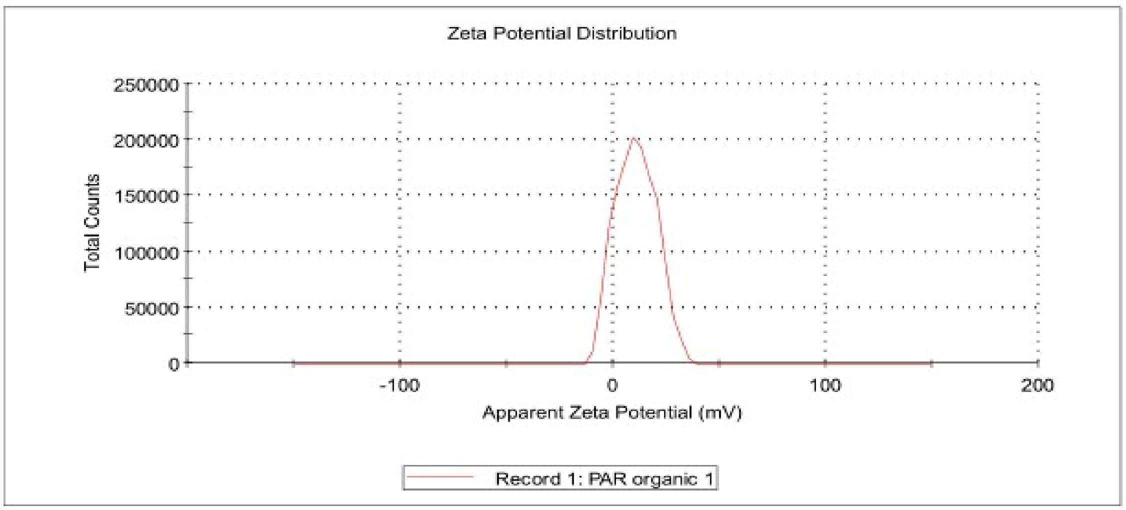

Fig.S1. Zeta Potential of PAR-Mg/Al LDH

Table S1: Remediation of various anionic dyes using MgAl LDHS and/or organic compounds prepared through different reported methods.

Adsorbent	Target dye	Qe (mg/g)	Ref
LDH modified with anionic surfactant (SDS-templated)	Methyl Orange (MO)	416.7	1
Mg–Al LDH (hydrothermal) — baseline study on anionic dye	Methyl Orange	148.3	2
MgAl-LDH	Methylene orange	197.62	3
MgAl-Charcoal activated	direct yellow	133.33	4

Pure Mg/Al-LDH	Reactive Brilliant Orange X-GN	≈79–83	[5]
CoAl-LDH	Acid fuchsin	384.62	[6]
PAR-Mg/Al LDH	**Acid fuchsin**	**568.18**	**Present work**

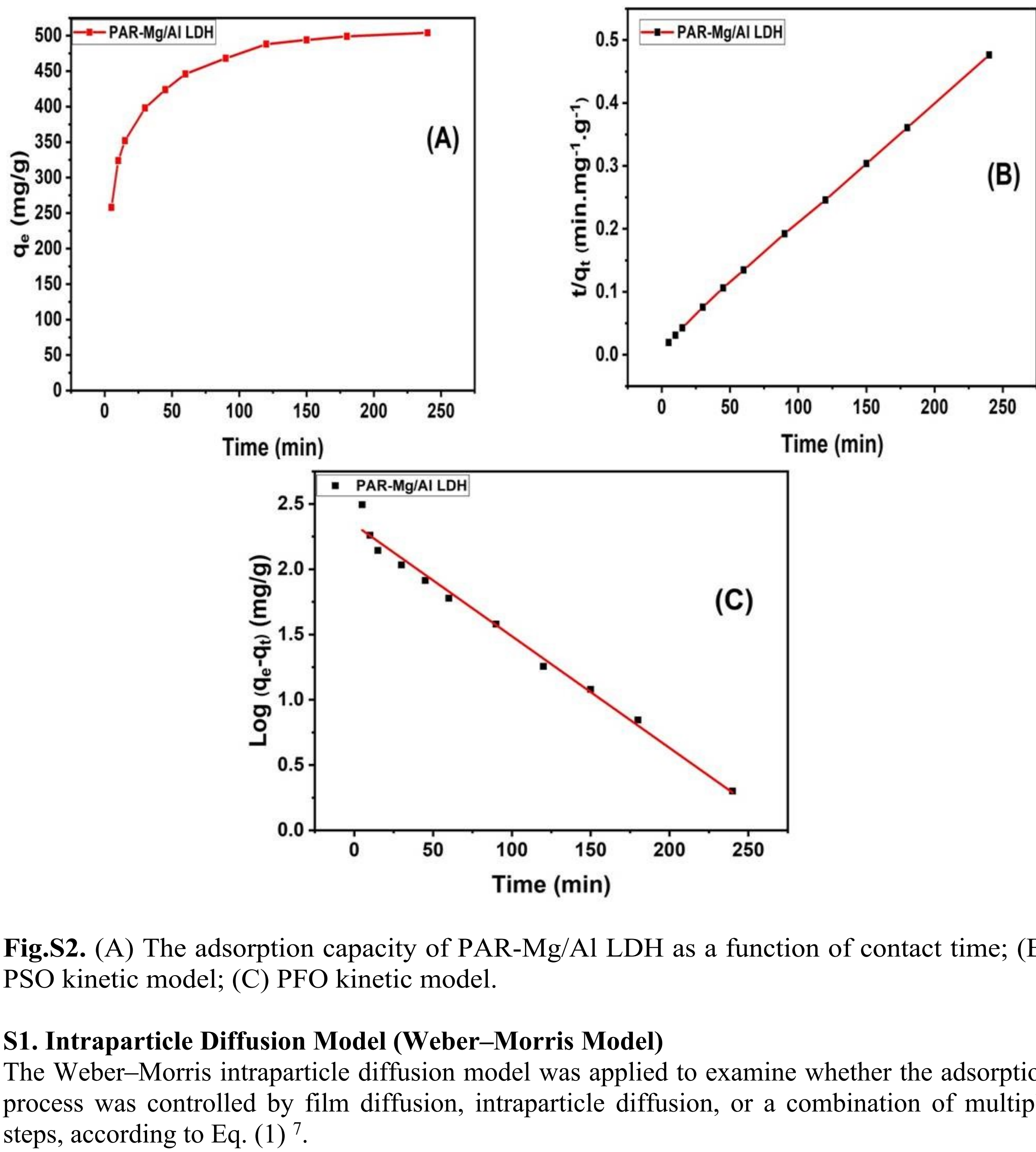

Fig.S2. (A) The adsorption capacity of PAR-Mg/Al LDH as a function of contact time; (B) PSO kinetic model; (C) PFO kinetic model.

S1. Intraparticle Diffusion Model (Weber–Morris Model)
The Weber–Morris intraparticle diffusion model was applied to examine whether the adsorption process was controlled by film diffusion, intraparticle diffusion, or a combination of multiple steps, according to Eq. (1) [7].

$$q_t = K_{id}\ t^{1/2} + C \qquad (1)$$

In this model, k_{id} (mg g^{-1} $h^{-0.5}$) represents the intraparticle diffusion rate constant, and *C* is a constant related to the thickness of the boundary layer. If intraparticle diffusion is involved in the adsorption process, a plot of q_t versus $t^{1/2}$ should yield a linear relationship. Furthermore, if intraparticle diffusion is the sole rate-limiting step, the plot should pass through the origin. The intercept *C* provides insight into the contribution of external mass transfer resistance, where higher *C* values indicate a greater boundary layer effect.

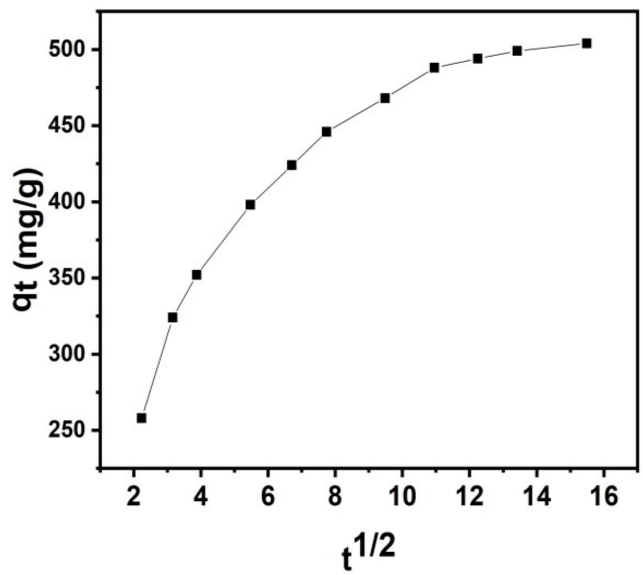

Fig. S3. Intraparticle diffusion plots for the adsorption of Acid Fuchsin on PAR-Mg/Al LDH.

S2. **Boyd Kinetic Model**:

To further distinguish between film diffusion and intraparticle diffusion as the rate-limiting step, the Boyd kinetic model was employed and is expressed by Eq. (2) [8].

$$F = 1 - \frac{6}{\Pi^2} \exp(1-Bt) \qquad (2)$$

In this model, *F* represents the fractional attainment of equilibrium at time *t*, and B_t is a function of *F*.

$$F = q_t/q_e \qquad (3)$$

Where q_t and $q_e$are the dye uptake (mmol g^{-1}) at time t and at equilibrium, respectively.
Eq. (2) can be rearranged to Eq. (4).[9]

$$B_t = -0.4977 - \ln(1-F) \qquad (4)$$

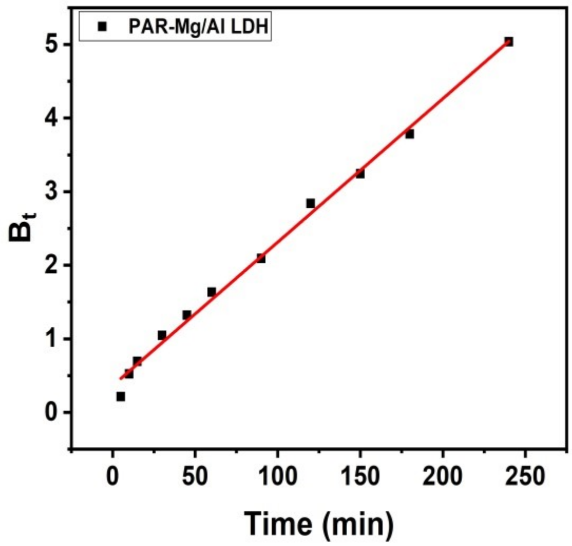

Fig. S4. Boyd plot (Bt versus t) for the adsorption of Acid Fuchsin on PAR-Mg/Al LDH.

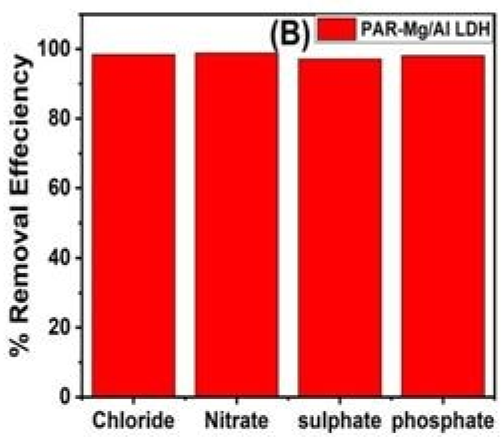

Fig.S5. Effect of interfering anions on acid fuchsin dye adsorption onto PAR-Mg/Al LDH.

Table S2. The docking interaction parameters of acid fuchsin with 7JWY: VIRAL PROTEIN / 7JWYCOVID -19.

	Ligand	Receptor	Interaction	Distance	E (Kcal/mol)
Shape A	N13 16 O	ASP 364 (A)	H-donor	3.22	-2.1

	O12 15 N	PHE 338 (A)	H-acceptor	3.38	-1.2		
Shape B	N13 16 O	CYC 336 (A)	H-donor	3.13	-0.7		
	O12 15 N	PHE 338 (A)	H-acceptor	3.05	-0.7		
	O12 15 N	GLY 339 (A)	H-acceptor	3.03	-4.4		
	6-ring CB	PHE 338 (A)	pi-H	4.04	-0.6		
	S	**rmsd**	**E_conf**	**E_place**	**E_score1**	**E_refine**	**E_score2**
1	-5.83096695	1.2215178	-145.591721	-89.7915039	-8.36091042	-29.4026527	-5.83096695
2	-5.69000053	1.69807434	-143.553314	-78.6248703	-8.49876308	-28.8788357	-5.69000053

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