Electronic Supporting Information

Sustainable Competitive Adsorption of Methylene Blue and Acid Red 88 from Synthetic Wastewater using NiO and/or MgO Silicate Based Nanosorbcats: Experimental and Computational Modeling Studies

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S1. Adsorption isotherms models

The experimental data were fitted using the Sips, Freundlich and Langmuir isotherm models for the single adsorption case. While the Extended-Sips model was used for binary systems. The models, assumptions, and the calculated coefficients are mentioned in Table S1.

S2. Single adsorption isotherms results

The adsorption experimental data were analyzed by different adsorption isothermal models. The model parameters for the single adsorption of the AR88 and MB molecules onto the SBNs are shown in **Table S2**. It is very clear from the calculations of χ^2 values that the Sips model better fits the experimental data than the Langmuir and Freundlich models. The χ^2 values for the applied Sips model ranged from 0.0058 to 0.0937 for MB and from 0.0720 to 0.0903 for AR88 in single systems.

Table S1. Adsorption isotherm models for single and multi-component (binary) systems.

Adsorption model	Nonlinear equation	Assumption(s)	Calculated coefficients	Reference
Langmuir	$Q_e = \frac{Q_m K_L C_e}{1 + K_L C_e}$	- Single adsorption system. - Homogenous surface. - The attraction between the adsorbed model molecules is negligible. - Constant adsorption energy at all sites.	- Q_e is the adsorption capacity at equilibrium $(mg\ g^{-1})$. - K_L is the Langmuir constant related to the binding sites $(L\ mg^{-1})$.	1
Freundlich	$Q_e = K_F C_e^{\ 1/n}$	- Single adsorption system. - Heterogonous surface. - The possibility of interaction between the adsorbed molecules. - Different adsorption energies of sites.	- K_F is the Freundlich constant related to the adsorption capacity $(mg\ g^{-1})(L\ mg^{-1})^{n-1}$ - $1/n$ is the adsorption intensity factor (unitless).	2
Sips	$Q_e = \frac{Q_m (K_s C_e)^{n_s}}{1 + (K_s C_e)^{n_s}}$	- Single adsorption system. - Used to predict the heterogeneous adsorption system circumventing the limitation of the rising adsorbate concertation associated with the Freundlich isotherm model.	- $Q_m is the$ maximum adsorbed amount $(mg\ g^{-1})$. - K_s is the Sips adsorption equilibrium constant $(L\ mg^{-1})$. - n_s is the Sips constant (unitless).	3, 4
Extended-Sips	$Q_e = \frac{Q_m (K_{si} C_{ei})^{n_{si}}}{1 + (K_{si} C_{ei})^{n_{si}} + (K_{sj} C_{ej})^{n_{sj}}}$	- Multi-component adsorption system. - It is a competitive form of the Sips isotherm used in the presence of another species.	- i and j represent the sorbate species.	5, 6

Table S2. Single adsorption isotherm parameters.

Model Molecule	SBNs	Langmuir isotherm		
		$Q_m\,(mg\,g^{-1})$	$K_L\,(L\,mg^{-1})$	χ^2
AR88	MgO	88.277	0.0308	1.6712
	NiO	64.851	0.0194	1.1441
	NiO-MgO	40.843	0.0849	3.7659
MB	MgO	43.317	0.0237	0.6551
	NiO	38.995	0.0911	1.8922
	NiO-MgO	47.399	0.0849	0.4373

Model Molecule	SBNs	Freundlich isotherm		
		K_f $(mg\,g^{-1})(L\,mg^{-1})^{n-1}$	n (unitless)	χ^2
AR88	MgO	6.429	0.49	0.7729
	NiO	4.243	0.47	0.4715
	NiO-MgO	7.301	0.32	0.1537
MB	MgO	2.682	0.53	0.0131
	NiO	6.925	0.35	0.1349
	NiO-MgO	8.509	0.37	0.3183

Model Molecule	SBNs	Sips isotherm			
		$Q_m\,(mg\,g^{-1})$	$K_s(L\,mg^{-1})$	n_s (unitless)	χ^2
AR88	MgO	147.2	0.0071	0.69	0.0720
	NiO	111.1	0.0039	0.66	0.0903
	NiO-MgO	137.7	0.0005	0.40	0.0840
MB	MgO	56.6	0.0111	0.80	0.0058
	NiO	69.4	0.0091	0.51	0.0082
	NiO-MgO	81.4	0.0164	0.57	0.0937

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