Supplementary Information (SI) for Environmental Science: Nano.
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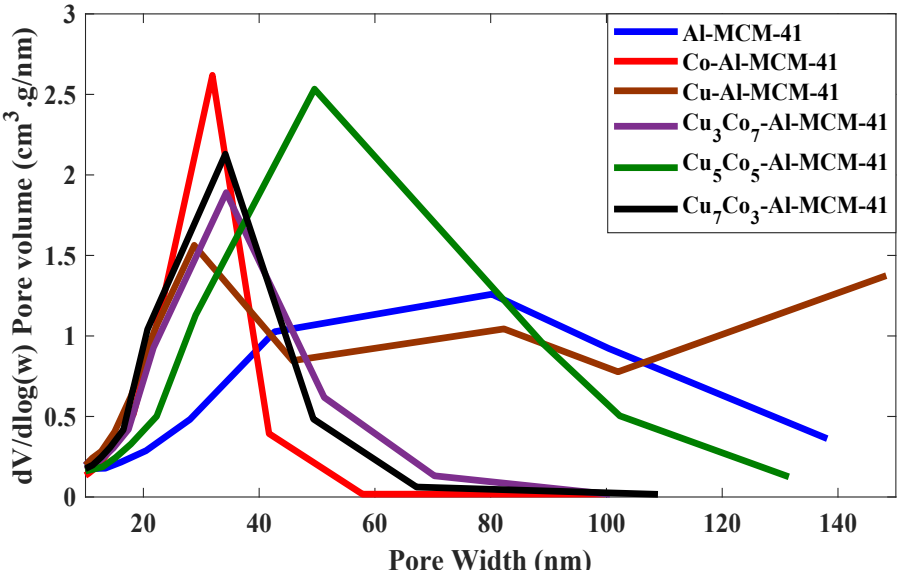


Figure S1: Textural porosity due to stacking of mesoporous particles in CuCo-Al-MCM-41

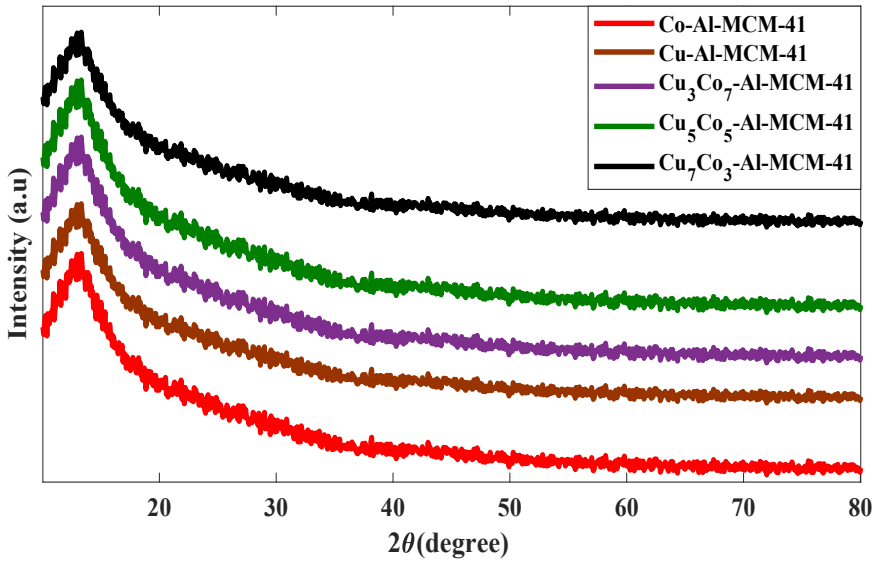


Figure S2: Large-angle XRD patterns of different Cu-Co-Al-MCM-41 nanostructures

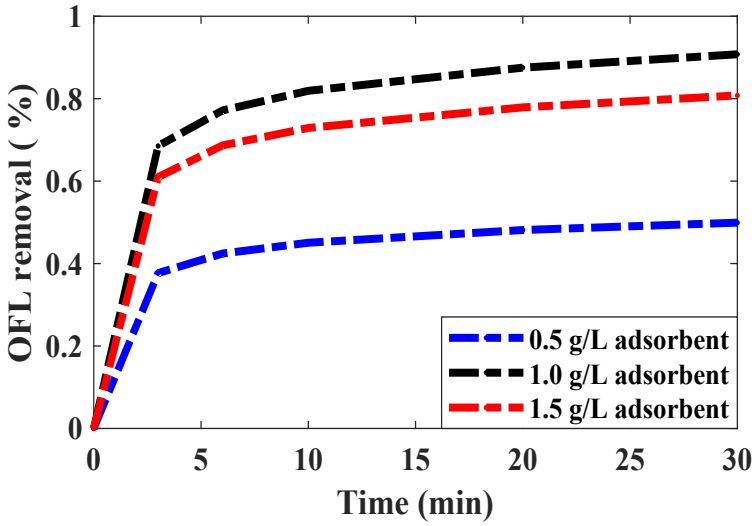


Figure S3: Effect of adsorbent (Cu_7Co_3-Al-MCM-41) dosage on the removal efficiency of OFL. Experimental Conditions: Initial concentration of OFL= 100 mg/L, temperature=room temperature (298 K), pH= 7.0

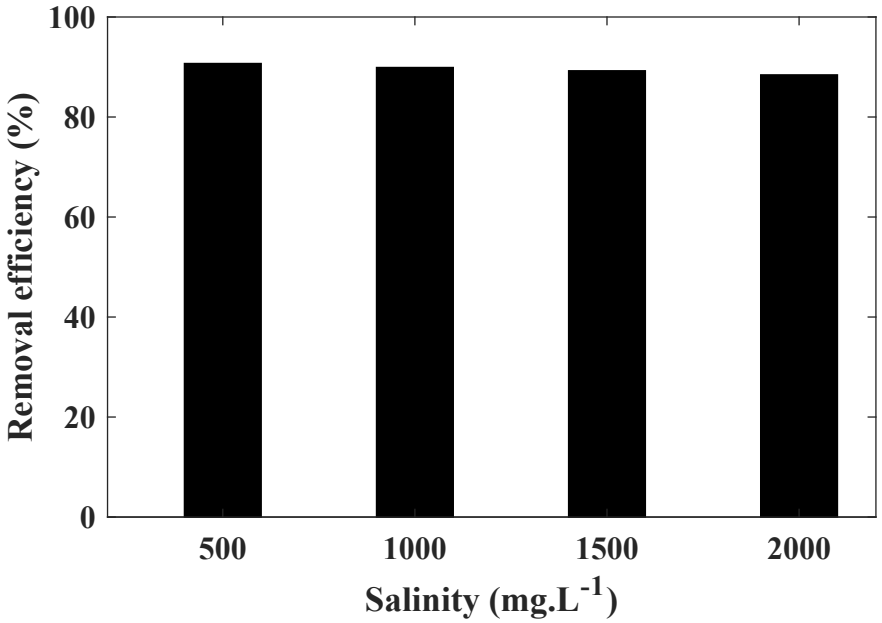


Figure S4: Effect of salinity on the removal efficiency of OFL: Experimental Conditions: Initial dosage of the adsorbent= 1.0 g/L, OFL concentration= 100 mg/L, temperature=room temperature (298 K), pH= 7.0, NaCl concentration: 500-2000 mg/L.

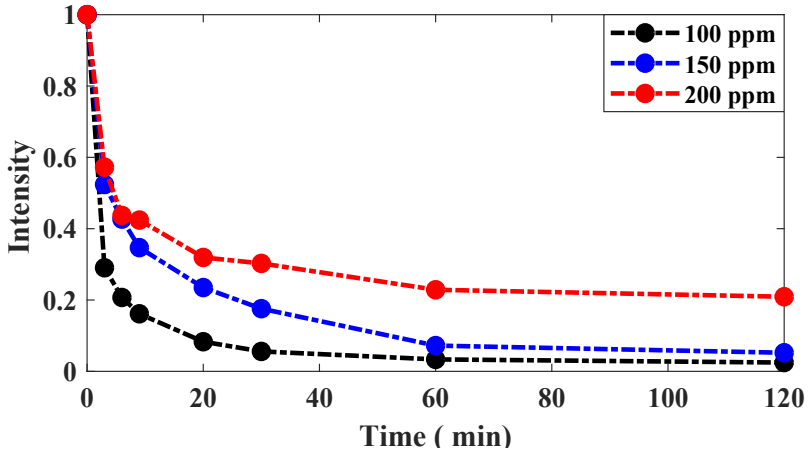


Figure S5: Raw kinetic data of adsorption at different initial OFL concentration. Experimental Conditions: dosage of the adsorbent= 1.0 g/L, temperature=room temperature (298 K), pH= 7.0

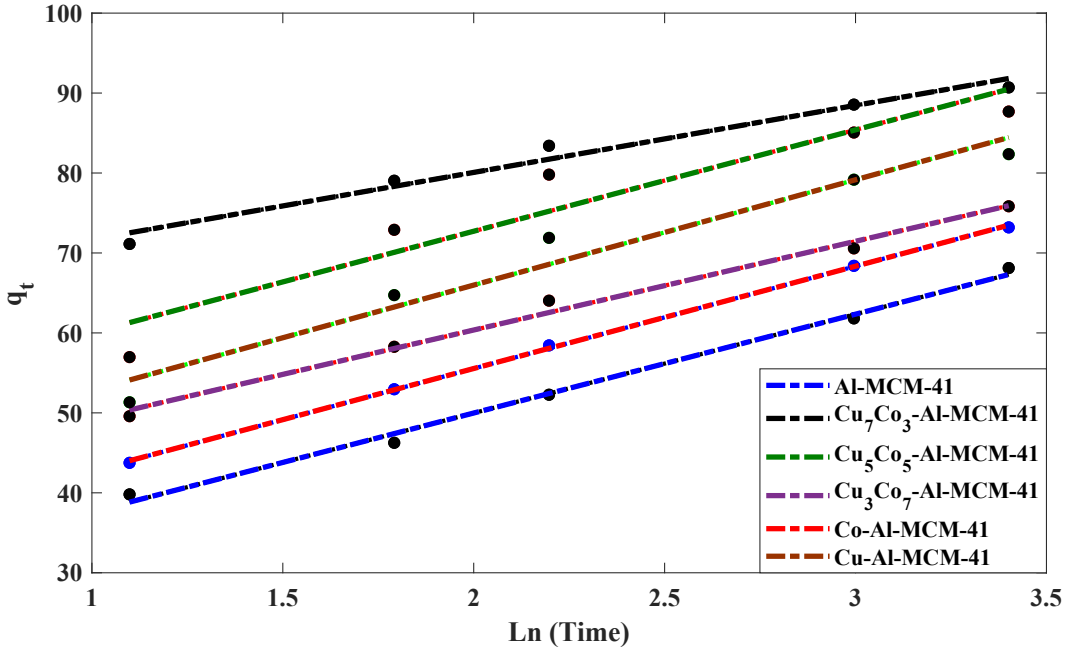
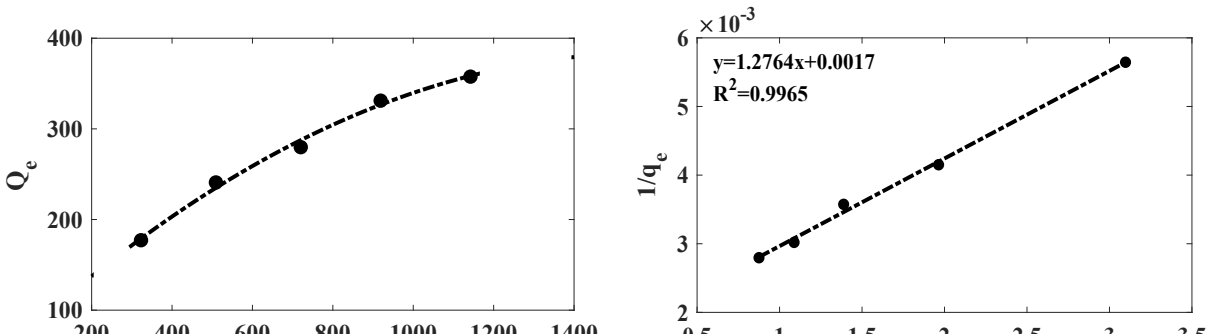


Figure S6: The Elovich equation fitted on data related to the effect of Cu-Co ratio on OFL adsorption, illustrating the role of aluminum and cobalt sites in chemisorption



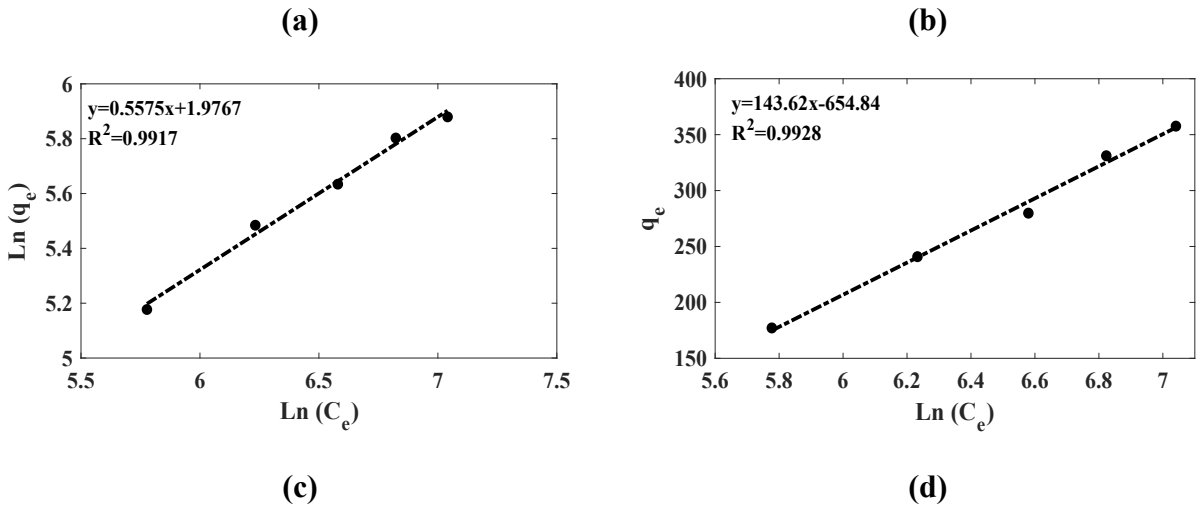


Figure S7: Various models fitted to the experimental data on OFL adsorption. **(a)** Experimental data **(b)** Langmuir isotherm, **(c)** Freundlich isotherm, and **(d)** Temkin isotherm.

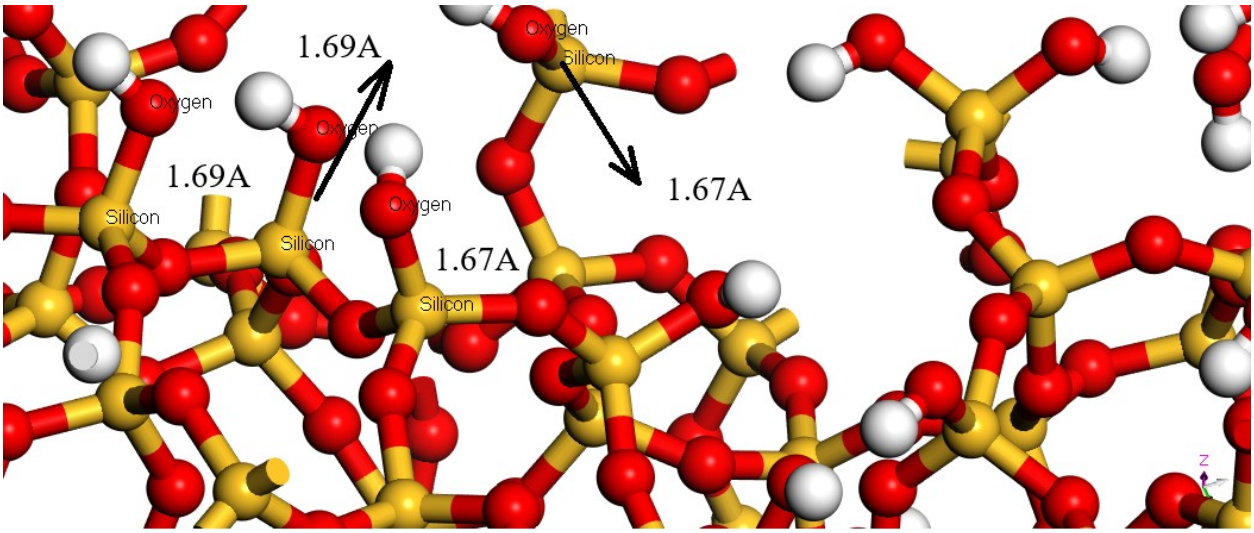


Figure S8. Optimized atomic structure of pure MCM-41 (side view) used in DFT calculations

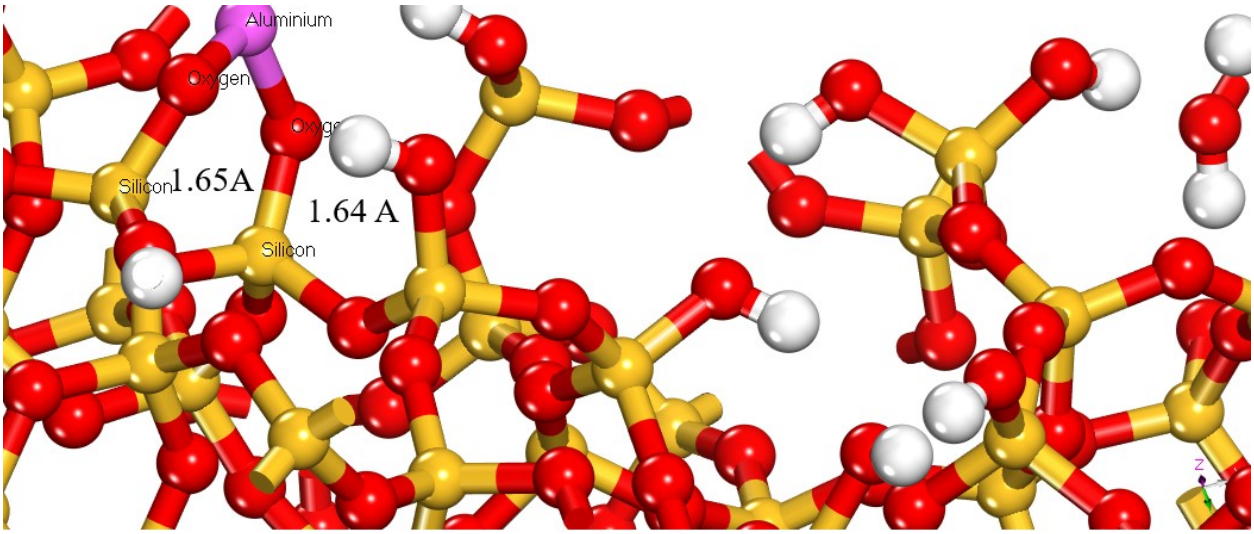


Figure S9- Optimized atomic structure of Al-MCM-41 (side view) used in DFT calculations

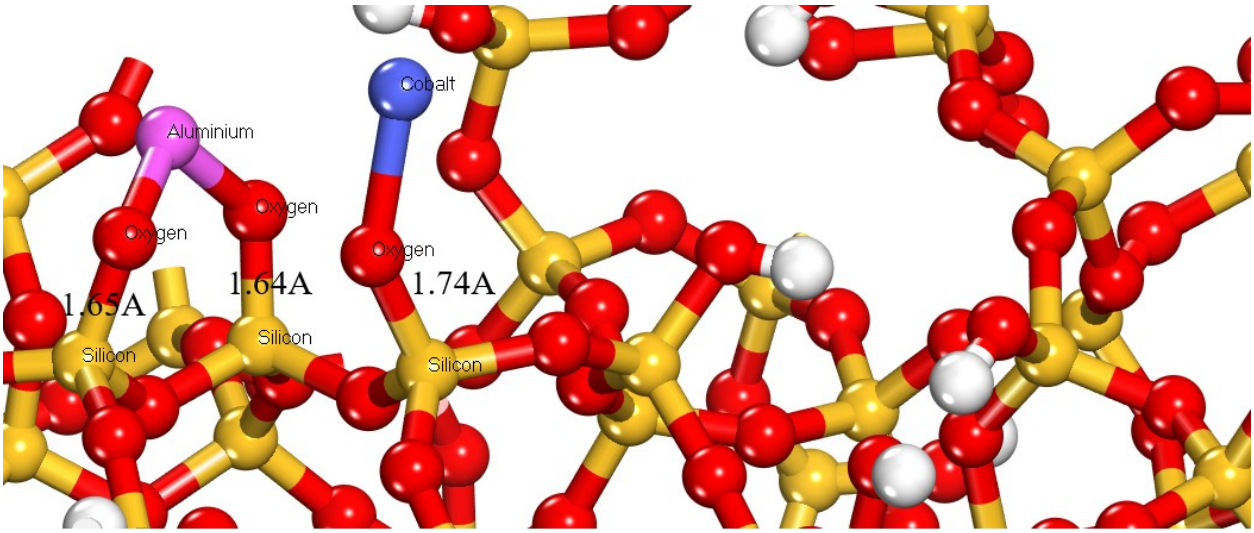


Figure S10. Optimized atomic structure of Co-Al-MCM-41 (side view) used in DFT calculations

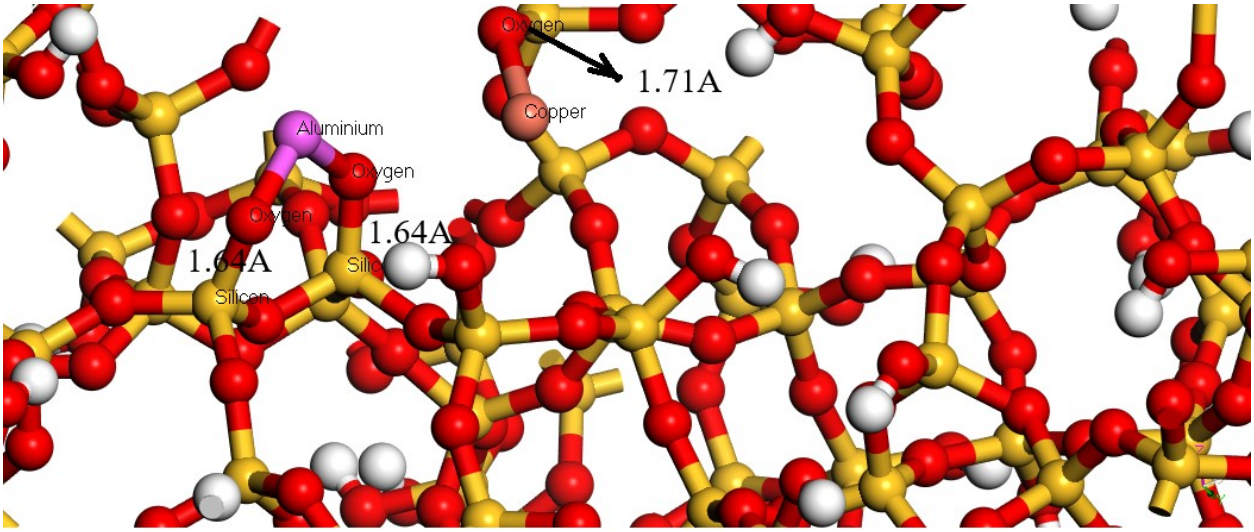


Figure S11. Optimized atomic structure of Cu-Al-MCM-41 (side view) used in DFT calculations

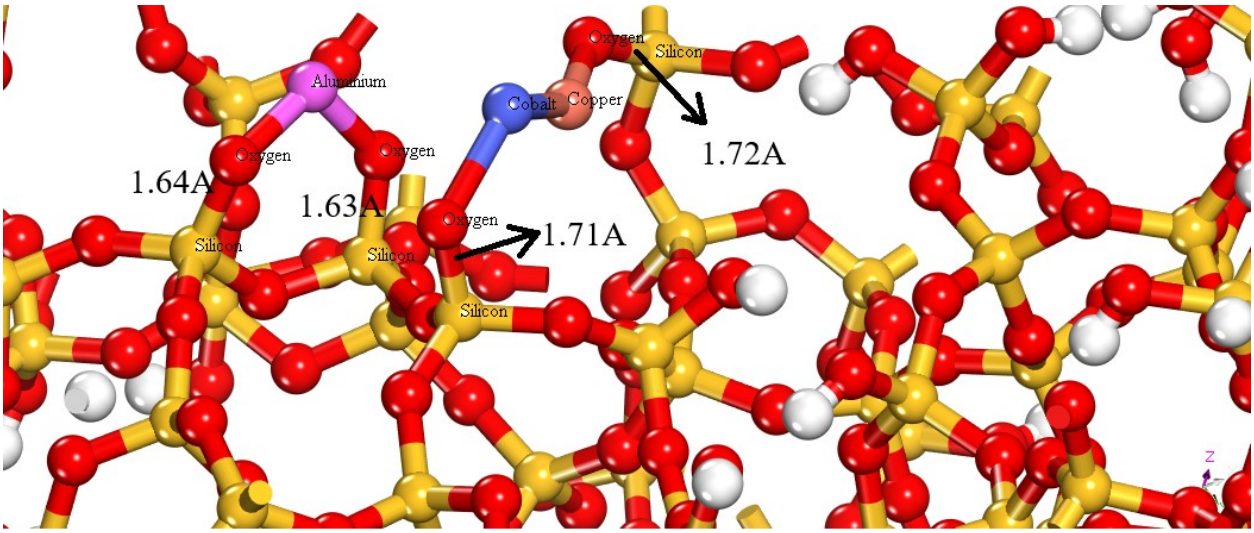


Figure S12. Optimized atomic structure of CuCo-Al-MCM-41 (side view) used in DFT calculations

Table S1. Adsorption kinetic parameters calculated from different kinetic models.

Model			**Adsorbent parameters**		
Pseudo-first order	**Conc(mg/L)**	q_e**(mg/g)***	q_e **(mg/g)****	$k_1\ (1/min)$	R^2
	100	97.53	1503	0.1347	0.967
	150	142.18	23933	0.1234	0.994
	200	158.16	19596	0.1101	0.980
Pseudo-second order	**Conc(mg/L)**	q_e **(mg/g)¹**	q_e **(mg/g)²**	$k_2\left(g/(mg.min)\right)$	R^2
	100	97.53	98.039	0.00737	0.999
	150	142.18	147.059	0.00151	0.997
	200	158.16	161.290	0.00191	0.998
Intra-particle diffusion	**Conc(mg/L)**	k_{b1} $(mg/(g.min^{0.5}))$	k_{b2} $(mg/(g.min^{0.5}))$	***C***	R^2
	100	20.35	1.908	24.716	0.999
	150	20.91	7.349	35.079	0.999
	200	23.61	5.704	45.566	0.984
Film diffusion model	**Conc(mg/L)**		$K_{FD}(1/min)$		R^2
	100		0.0585		0.967
	150		0.0536		0.994
	200		0.0487		0.984
Elovich equation model	**Conc(mg/L)**		$\alpha\left((mg.min)/g\right)$	$\beta(g/mg)$	R^2
	100		272.09	0.0980	0.859
	150		263.34	0.0493	0.979
	200		623.87	0.0498	0.966

$*q_e$ (mg/g) represents the experimental adsorption capacity, ** q_e (mg/g) represents the theoretical adsorption capacity. The parameters k_1 , k_2, K_{b1} & K_{b2} , and K_{FD} correspond to the rate constants for the PFO, PSO, IPD, and FDM, respectively. Additionally, *C* is the intra-particle constant, which reflects the boundary layer's thickness. The parameters α and β represent the initial adsorption and desorption constants, respectively.

Table S2. Mulliken atomic charges difference before and after adsorption in absorbent and OFL.

Adsorbent	ΔCh_{Al}	ΔCh_{Cu}	ΔCh_{Co}	ΔCh_{o} (OFL)	ΔCh_{C} (OFL)
Al-MCM-41	+0.17	---	---	-0.13	0.00
Co-Al-MCM-41	+0.39	---	+0.05	-0.22	-0.07
Cu-Al-MCM-41	+0.33	0.00	---	-0.15	0.00
CuCo-Al-MCM-41	+0.54	+0.02	+0.14	-0.30	-0.10

ΔCh_{Al} , represent the Mulliken atomic charges difference of Al before and after adsorption in adsorbent and OFL.
ΔCh_{Cu} , represent the Mulliken atomic charges difference of Cu before and after adsorption in adsorbent and OFL.
ΔCh_{Co} , represent the Mulliken atomic charges difference of Co before and after adsorption in adsorbent and OFL
ΔCh_{o} (OFL), represent the Mulliken atomic charges difference of Oxygen in Ofloxacin before and after adsorption in absorbent and OFL
ΔCh_{C} (OFL), represent the Mulliken atomic charges difference of Carbon in Ofloxacin before and after adsorption in absorbent and OFL