Electronic Supplementary Information

Cationic dye adsorption and separation at discrete molecular level: First example of an iron cluster with rapid and selective adsorption of methylene blue from aqueous system

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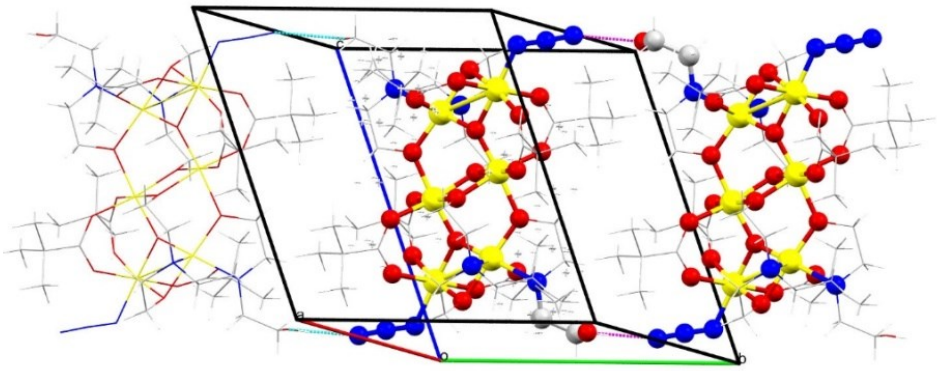

Fig. S1 Packing view for **1.**

Table S1. Selected Bond Distances (Å) and Angles (°) for **1**.

Distances (Å)			
Fe_1-O_1	1.9094(16)	Fe_1-O_2	2.0512(17)
Fe_1-O4	1.9610(16)	Fe_1-O_5	2.0632(18)
Fe_2-O_1	1.9248(16)	Fe_2-O_2	2.0453(17)
Fe_2-O_3	2.0201(18)	Fe_2-O_6	2.0374(18
Fe_2-O_{10}	2.0602(18)	Fe_3-O	1.8689(16)
Fe_3-O_4	2.0414(15)	Fe_3-O_7	2.0398(17)
Fe_3-O'_7	2.0144(17)	Fe_3-O_9	2.0444(18)

Angles (°)			
Fe_1-O_1-Fe_2	101.92(7)	Fe_3-O_1-Fe_1	124.25(9)
Fe_3-O_1-Fe_2	124.00(9)	Fe_1-O_4-Fe_3	119.66(8)
Fe_3-O_7-Fe_3	102.06(8)		

Table S2: Parameters for different kinetic models for adsorption studies of MB and MO.

Model		**Pseudo-first order**				**Pseudo-second order**				**Intraparticle diffusion**	
Parameter		k_1 (min^{-1})	q_e (cal) (mg/g)	q_e (exp) (mg/g)	R^2	k_2 ($gmg^{-1}min^{-1}$)	q_e (cal) (mg/g)	q_e (exp) (mg/g)	R^2	K_p ($mg\ g^{-1}min^{-1/2}$)	R^2
1	**MB**	0.091	68.52	88.68	0.972	0.011	102.28	88.68	0.999	10.61	0.865
	MO	0.071	53.21	49.30	0.966	0.003	55.55	49.30	0.986	6.527	0.715