Supplementary material

Fabrication of amino functionalized benzene-1,4-dicarboxylic acid facilitated cerium based metal organic frameworks for efficient removal of fluoride from water environment

Antonysamy Jeyaseelan[1], Mu. Naushad[2,3], Tansir Ahamad[2], Natrayasamy Viswanathan[1*]

[1]Department of Chemistry, Anna University, University College of Engineering - Dindigul, Dindigul – 624 622, Tamilnadu, India.

[2]Department of Chemistry, College of Science, King Saud University, Riyadh-11451, Saudi Arabia.

[3]Yonsei Frontier Lab, Yonsei University, Seoul, Korea.

Corresponding author. Tel.: +91-451-2554066 (O); fax: +91-451-2554066.

E-mail address: drnviswanathan@gmail.com (N. Viswanathan)

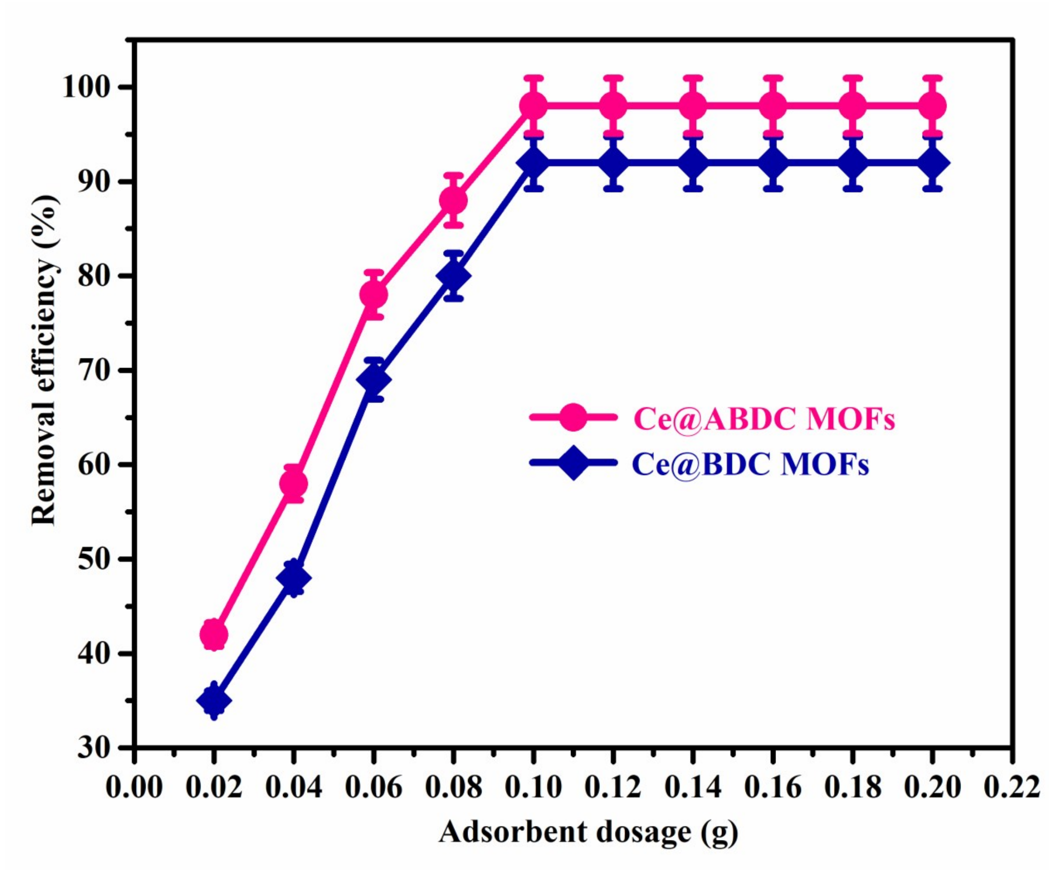

Fig. S1. Effect on adsorbent dosage on removal efficiency of fluoride by Ce-based MOFs.

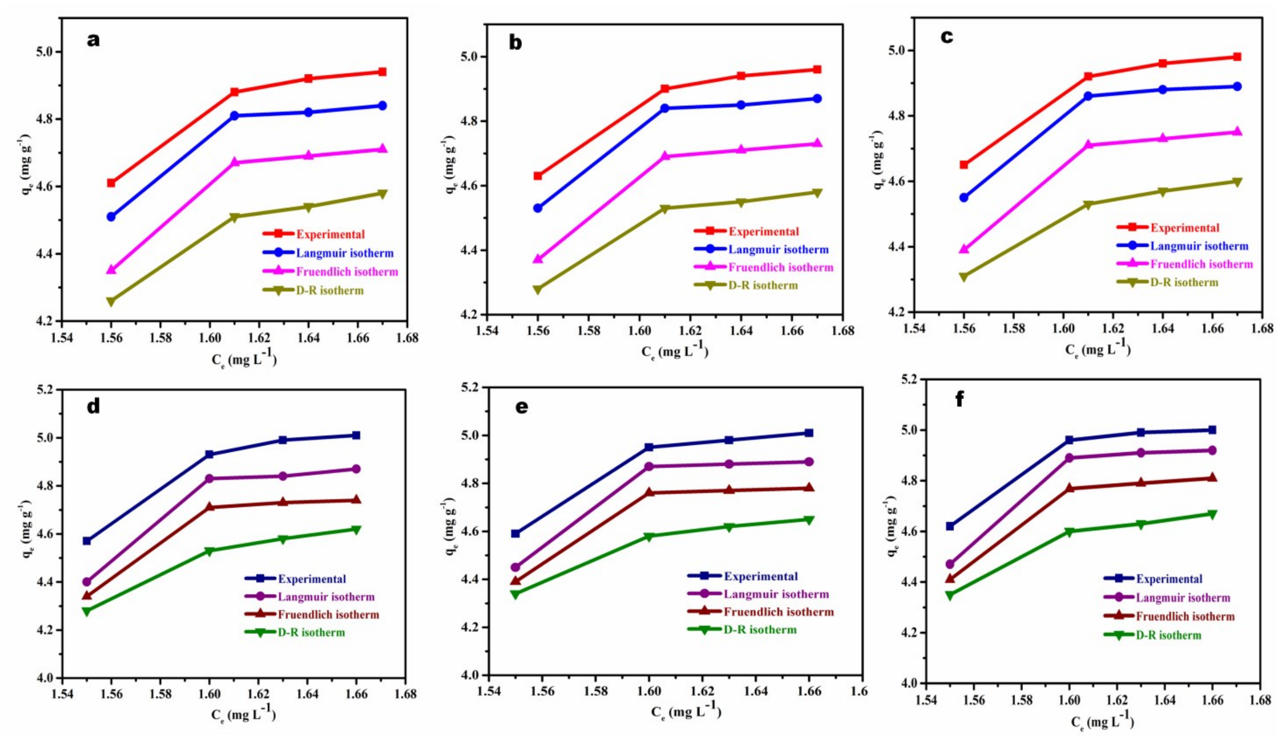

Fig. S2. Fluoride adsorption isotherms (C_e vs q_e) of (a-c) Ce@BDC MOFs at 303, 313 and 323 K and (d-f) Ce@ABDC MOFs at 303, 313 and 323 K.

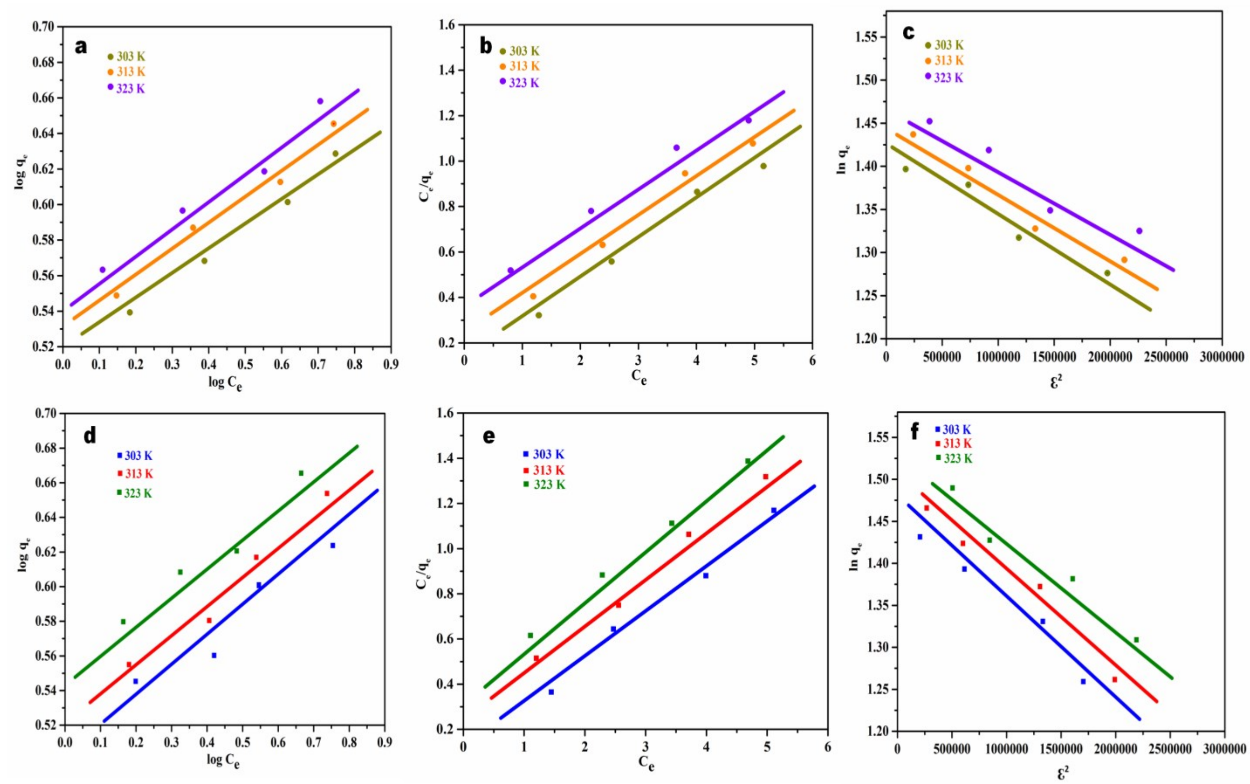

Fig. S3. The linear plots of (a) Fruendlich; (b) Langmuir; (c) Dubinin-Raduskevich adsorption isotherm models of Ce@BDC MOFs towards fluoride adsorption at 303, 313 and 323 K; The linear plots of (d) Fruendlich; (e) Langmuir; (f) Dubinin-Raduskevich adsorption isotherm models of Ce@ABDC MOFs towards fluoride adsorption at 303, 313 and 323 K.

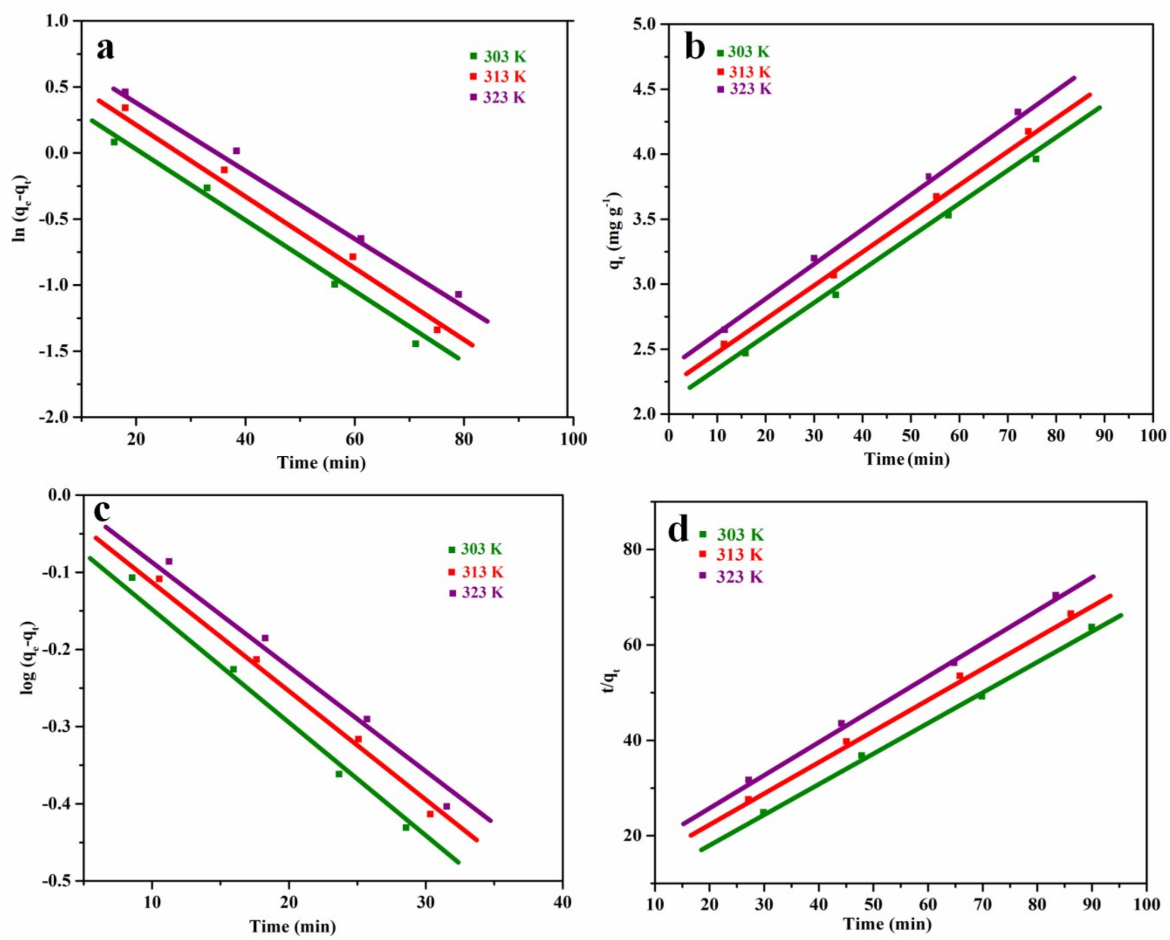

Fig. S4. Kinetic linear plots of (a) pseudo-first-order; (b) pseudo-second-order kinetic models; (c) particle diffusion and (d) intraparticle diffusion model of the Ce@BDC MOFs towards defluoridation at 303, 313 and 323 K.

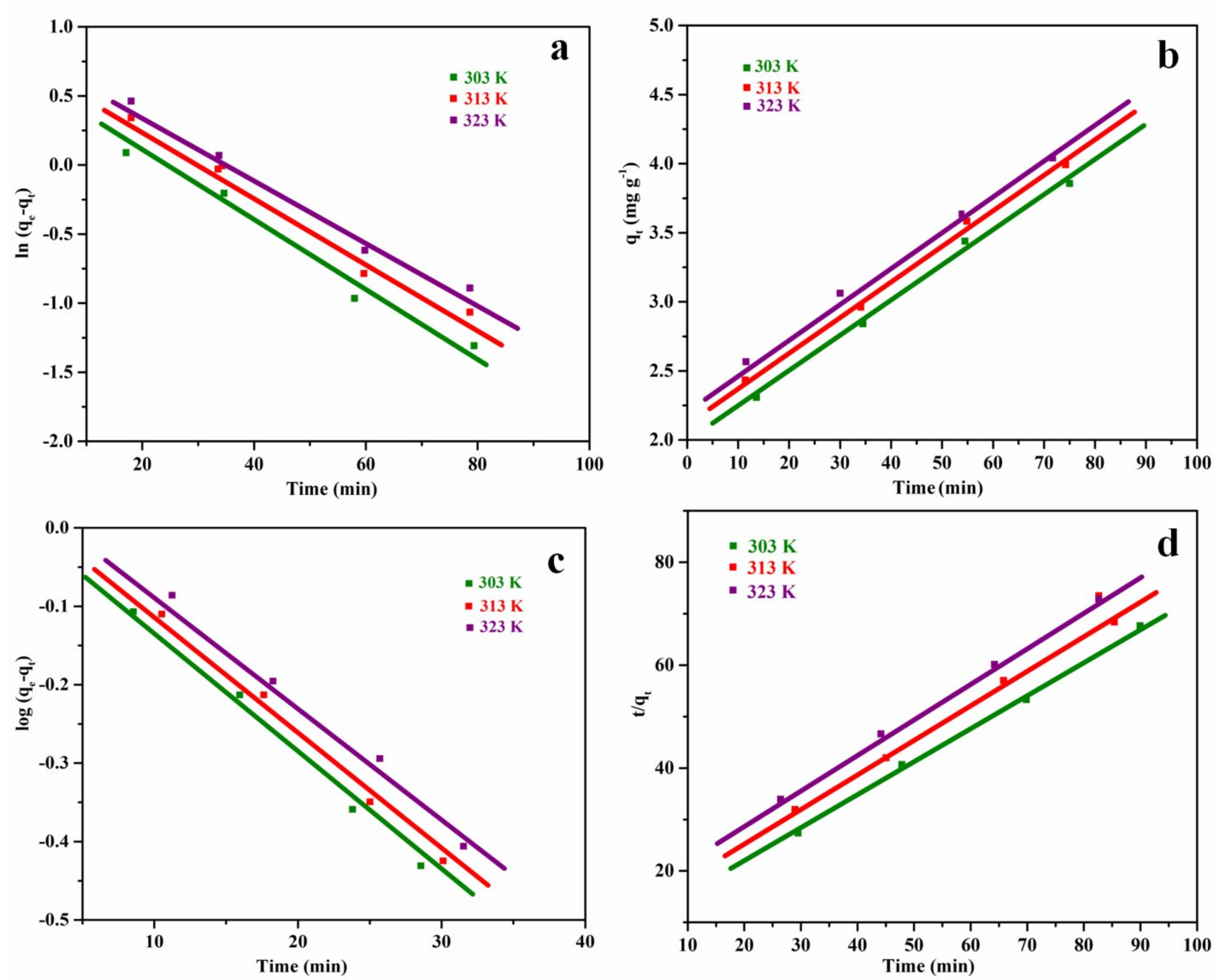

Fig. S5. Kinetic linear plots of (a) pseudo-first-order; (b) pseudo-second-order kinetic models; (c) particle diffusion and (d) intraparticle diffusion model of the Ce@ABDC MOFs towards defluoridation at 303, 313 and 323K.

Table S1. Kinetic studies of Ce@BDC MOFs towards defluoridation.

Kinetic models	Parameters	303 K				313 K				323 K			
		8 mg/L	10 mg/L	12 mg/L	14 mg/L	8 mg/L	10 mg/L	12 mg/L	14 mg/L	8 mg/L	10 mg/L	12 mg/L	14 mg/L
Pseudo-first-order	$k_{ad}(min^{-1})$	0.105	0.112	0.121	0.128	0.109	0.118	0.124	0.131	0.113	0.121	0.129	0.135
	r	0.885	0.892	0.900	0.909	0.888	0.896	0.904	0.913	0.892	0.899	0.906	0.917
	sd	0.318	0.324	0.329	0.333	0.320	0.327	0.332	0.337	0.324	0.330	0.335	0.340
Pseudo-second-order	$q_e(mg\ g^{-1})$	4.950	4.954	4.957	4.960	4.952	4.957	4.968	4.972	4.953	4.959	4.961	4.973
	$k\ (g\ mg^{-1}\ min^{-1})$	0.295	0.301	0.310	0.316	0.298	0.305	0.313	0.320	0.300	0.308	0.316	0.323
	$h\ (mg\ g^{-1}\ min^{-1})$	2.238	2.243	2.248	2.252	2.241	2.246	2.250	2.255	2.444	2.248	2.253	2.259
	r	0.975	0.981	0.988	0.992	0.978	0.983	0.990	0.993	0.980	0.985	0.992	0.995
	sd	0.134	0.139	0.146	0.153	0.138	0.142	0.150	0.156	0.141	0.146	0.153	0.159
Particle diffusion	$k_p(min^{-1})$	0.208	0.215	0.222	0.228	0.212	0.219	0.226	0.231	0.216	0.222	0.229	0.234
	r	0.866	0.873	0.877	0.882	0.870	0.875	0.880	0.886	0.872	0.879	0.883	0.890
	sd	0.408	0.413	0.419	0.423	0.411	0.417	0.421	0.426	0.413	0.420	0.424	0.430
Intra particle diffusion	$k_i(mg\ g^{-1}\ min^{0.5})$	1.124	1.135	1.142	1.149	1.129	1.138	1.146	1.154	1.133	1.142	1.150	1.157
	r	0.954	0.963	0.969	0.975	0.959	0.966	0.973	0.978	0.963	0.971	0.977	0.983
	sd	0.128	0.135	0.142	0.148	0.133	0.139	0.146	0.152	0.137	0.142	0.149	0.157

Table S2. Kinetic studies of Ce@ABDC MOFs towards defluoridation.

Kinetic models	Parameters	303 K				313 K				323 K			
		8 mg/L	10 mg/L	12 mg/L	14 mg/L	8 mg/L	10 mg/L	12 mg/L	14 mg/L	8 mg/L	10 mg/L	12 mg/L	14 mg/L
Pseudo-first-order	k_{ad}(min^{-1})	0.124	0.132	0.139	0.146	0.127	0.136	0.143	0.155	0.132	0.141	0.148	0162
	r	0.928	0.937	0.943	0.949	0.932	0.940	0.946	0.952	0.935	0.943	0.949	0.955
	sd	0.346	0.351	0.355	0.359	0.348	0.354	0.357	0.363	0.351	0.356	0.361	0.366
Pseudo-second-order	q_e(mg g^{-1})	4.913	4.918	4.921	4.923	4.915	4.920	4.922	4.925	4.917	4.921	4.924	4.928
	k (g mg^{-1} min^{-1})	0.412	0.423	0.431	0.439	0.417	0.426	0.434	0.442	0.421	0.429	0.437	0.446
	h (mg g^{-1} min^{-1})	2.375	2.384	2.389	2.396	2.379	2.387	2.392	2.401	2.383	2.391	2.396	2.405
	r	0.978	0.982	0.987	0.993	0.981	0.985	0.988	0.995	0.984	0.987	0.991	0.997
	sd	0.139	0.144	0.149	0.152	0.141	0.146	0.151	0.155	0.144	0.148	0.154	0.198
Particle diffusion	k_p(min^{-1})	0.194	0.201	0.207	0.214	0.198	0.205	0.211	0.219	0.201	0.209	0.214	0.222
	r	0.915	0.925	0.934	0.942	0.918	0.929	0.937	0.946	0.922	0.931	0.940	0.949
	sd	0.410	0.414	0.418	0.422	0.412	0.417	0.420	0.425	0.415	0.419	0.423	0.429
Intra particle diffusion	k_i(mg g^{-1} min$^{0.5}$)	1.758	1.765	1.771	1.776	1.762	1.768	1.774	1.779	1.765	1.771	1.776	1.781
	r	0.981	0.986	0.990	0.994	0.983	0.988	0.993	0.996	0.987	0.991	0.995	0.998
	sd	0.125	0.138	0.142	0.145	0.129	0.141	0.144	0.147	0.131	0.142	0.146	0.149