Supplementary Information (SI) for CrystEngComm.

Supporting Information

Rapid and efficient Sr(II) capture by lanthanide-clusters based metal-organic frameworks containing alkali metal ions

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1. Equations for ion exchange analysis

The equations for ion exchange analysis are summarized as follows:

(1) Removal rate (R %)

$$R = \frac{(C_0 - C_e)}{C_0} \times 100\% \quad \text{(Eq. S1)}$$

Here, C_0 (mg/L) and C_e (mg/L) are the initial concentration and equilibrium concentration of metal ions, respectively, which can be measured by ICP.

(2) Distribution coefficient (K_d)

$$K_d = \frac{V}{m}\frac{(C_0 - C_e)}{C_e} \quad \text{(Eq. S2)}$$

Where C_0 (mg/L) and C_e (mg/L) are the initial and equilibrium concentrations of the target ion, respectively; m (g) and V (mL) are the mass of the adsorbent material and the volume of the solution used in the ion exchange experiment, respectively.

(3) Kinetics model

$$ln\frac{(q_e - q)}{q_e} = -k_1 t \quad \text{(Eq. S3a)}$$

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e} \quad \text{(Eq. S3b)}$$

Here, q_e and q_t are the amounts of Sr^{2+} ions adsorbed (mg/g) at equilibrium and at time t, respectively; t is the adsorption time (min); k_1 is the pseudo-first-order rate constant of adsorption (min^{-1}) and k_2 is the pseudo-second-order rate constant of adsorption (g/mg/min).

(4) The adsorption capacity q

$$q = \frac{(C_0 - C_e)V}{m} \quad \text{(Eq. S4)}$$

Here, V (mL) is the volume of the solution used in the ion exchange experiment, and m (g) is the mass of the adsorbent material.

(5) Adsorption isotherm models

$$q = q_m \frac{bC_e}{1 + bC_e} \quad \text{(Eq. S5a)}$$

$$q = q_m \frac{(bC_e)^{1/n}}{1 + (bC_e)^{1/n}} \quad \text{(Eq. S5b)}$$

$$q = kc_e^{1/n} \quad \text{(Eq. S5c)}$$

Where q (mg/g) is the number of ions adsorbed per unit weight of the adsorbent at the equilibrium concentration C_e (mg/L) q_m is the maximum adsorption capacity, and b (L/mg) is the Langmuir constant related to the free energy of adsorption, n is a constant that characterizes the heterogeneity of the system.

(6) The desorption rate can be considered as the percentage of the mass of Sr^{2+} ions desorbed off to the mass of Sr^{2+} ions adsorbed on, but considering the loss of solid mass, it can be calculated by the following equation:

$$E = \frac{C_e^{de} V_{de}}{m_2 (m_{Sr}^{ad} / m_{ad})} \times 100\% \quad \text{(Eq. S6)}$$

where C_e^{de} (mg/L) is the Sr^{2+} concentration in the solution after desorption, V_{de} (L) is the volume of solution used during desorption. M_{Sr}^{ad} (mg) is the mass of adsorbed Sr^{2+} ion during the adsorption process, and m_{ad} (mg) is the mass of the solid sample after adsorption of Sr^{2+}, m_2 (mg) is the mass of the solid sample used during desorption.

(7) Separation factor (*SF*)

$$SF = \frac{K_d^A}{K_d^B} \quad \text{(Eq. S7)}$$

In this equation, K_d^A and K_d^B represent the distribution coefficients of A and B ions, respectively.

2. Characterization techniques

Powder X-ray diffraction (PXRD) patterns were recorded in the angular range of $2\theta = 5 - 65^{\circ}$ on a Rigaku Miniflex II diffractometer with CuKα radiation (λ = 1.54178 Å). Elemental analyses (EA) of N, C, and H were conducted with the German Elementary Vario EL III instrument. Thermogravimetric analysis (TGA) was performed on a Netzsch STA449C instrument, from room temperature to 800 °C, under N_2 atmosphere, at a heating rate of 10 °C/min. Energy spectrum (EDS), element distribution map, and scanning electron microscope (SEM) images were obtained on the JEOL JSM-6700F scanning electron microscope. X-ray photoelectron spectroscopy (XPS) analysis was performed on the ThermoFisher ESCALAB 250Xi XPS spectrometer; all peaks were corrected to the binding energy of the C1s peak of adventitious carbon at 284.8 eV. Inductively coupled plasma mass spectrometry (ICP-MS) was performed on XSeries II, and inductively coupled plasma optical emission spectroscopy (ICP-OES) was performed on Thermo 7400. pH values of all solutions were tested by Shanghai Leach E-201F. In the γ irradiation experiments, samples were irradiated at an irradiation dose rate of 1.2 kGy/h for 89 h and 175 h (total irradiation dose of 100 kGy and 200 kGy). The γ-ray irradiation was provided by the ^{60}Co irradiation source in Suzhou CNNC Huadong Radiation Co., Ltd, China. The pH values of all solutions were measured by Shanghai Leich E-201 F.

3. Ion exchange experiments

(1) **Adsorption Kinetics.** 50 mg sample of **K-Dy** or **Na-Dy** powder was weighed and added to 50 mL of a Sr^{2+} ion solution with an initial concentration of approximately 5 mg/L. The mixture was subjected to magnetic stirring at room temperature. At specific time intervals (1, 2, 3, 5, 10, 20, 30, 60, 90, 120, 180, 300, 360, 480, and 600 min), approximately 2 mL of the solution was withdrawn and filtered. The filtered samples were then diluted for subsequent determination of the Sr^{2+} ion concentration.

(2) **Adsorption Isotherms.** The **K-Dy** or **Na-Dy** samples were ground into a uniform powder. A 10 mg powder sample was mixed with 10 mL of Sr^{2+} ion solutions of varying concentrations (approximately 5 - 800 mg/L). The mixtures were stirred at room temperature for 8 hours. The supernatant was collected and filtered using a syringe filter. The filtrate was then diluted with a 2% HNO_3 aqueous solution to an appropriate concentration for the subsequent determination of the Sr^{2+} ion concentration.

(3) **The effect of pH on Sr^{2+} adsorption.** The pH of the Sr^{2+} ion solution was adjusted to a range of 2.97 to 11.84 using HNO_3 or NaOH solutions, with the final concentration of Sr^{2+} ions maintained at approximately 5 mg/L. A 10 mg sample of **K-Dy** powder was sequentially added to 10 mL of the Sr^{2+} ion solution at each pH value. The mixtures were subjected to magnetic stirring at room temperature for 8 hours. After the reaction, approximately 2 mL of the supernatant was collected. The remaining suspension was separated by centrifugation to isolate the powder samples.

(4) **The effect of irradiation on Sr^{2+} adsorption.** The **K-Dy** and **Na-Dy** samples were irradiated with γ-rays at 1.2 kGy/h to expose them to γ-irradiation at a dose of 100 or 200 kGy. Subsequently, 10 mg of the original **K-Dy** and **Na-Dy** samples and their irradiated samples were weighed and powdered, and then added into 10 mL of 5 mg/L Sr^{2+} ion solution respectively, and stirred for 8 h at room temperature.

(5) **Elution and reuse.** 200 mg of **K-Dy** was added to 200 mL of 5 mg/L aqueous Sr^{2+} ion solution

and stirred at room temperature for 4 h. The remaining solid sample was washed with deionised water and anhydrous ethanol, dried naturally, and weighed. The product after Sr^{2+} ion exchange was then eluted with 0.5 M KCl solution with stirring for 12 h. The solid sample was washed and dried naturally to obtain the eluted sample. The sample was cycled three times, and the concentration of Sr^{2+} ions in the solution was determined after each cycle, and the cycled sample was subjected to PXRD test.

(6) **Competitive adsorption.** Initially, mixed solutions containing Sr^{2+} ions along with other metal ions (Na^{+}, Cs^{+}, Ca^{2+}, and Mg^{2+}) were prepared, including both single-component and multi-component mixtures. Additionally, low-concentration Sr^{2+} ions (approximately 5 mg/L) were artificially added to tap water (from Fuzhou, China) and river water (from the Wulong River in Fuzhou) to simulate real water samples contaminated with radioactive strontium.

4. Crystal structure

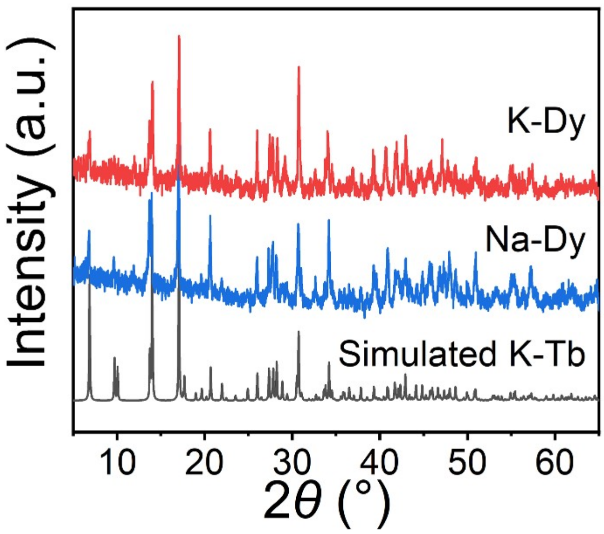

Figure S1. PXRD patterns of K-Dy and Na-Dy samples compared with the simulated one from single crystal data of K-Tb.

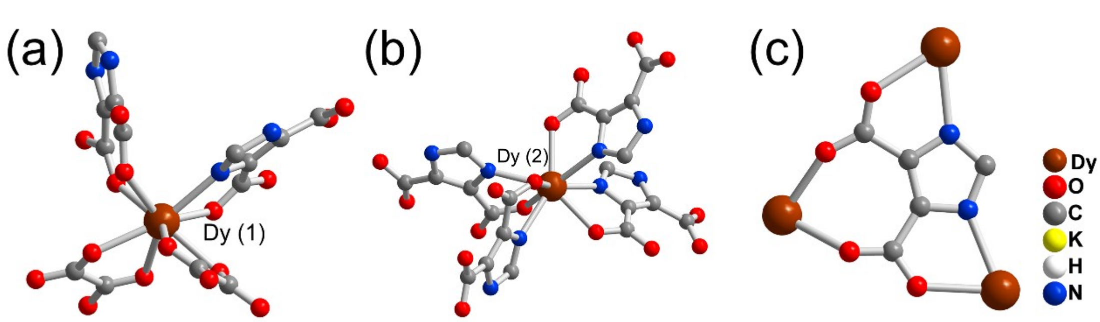

Figure S2. The coordination modes of Dy^{3+} ions (a, b) and IDC^{3-} (c) in **K-Dy**.

Table S1. Elemental analysis results for **K-Dy**, **K-Dy-Sr**, **Na-Dy**, and **Na-Dy-Sr**.

	K-Dy	**K-Dy-Sr**	**Na-Dy**	**Na-Dy-Sr**

	theoretical	actual	theoretical	actual	theoretical	actual	theoretical	actual
C	14.41	15.74	14.27	15.17	14.93	15.10	14.27	13.38
H	1.89	2.22	1.87	2.53	1.95	2.43	1.87	2.24
N	4.80	5.12	4.75	4.78	4.97	4.84	4.75	3.97

5. Sr^{2+} Adsorption Kinetics

Table S2. The Sr^{2+} adsorption kinetics results of **K-Dy** (V/m = 1000 mL/g; at room temperature (RT)).

Time (minute)	C_t (mg/L)	q (mg/g)	R^{Sr} (%)	K_d^{Sr} (mL/g)
0	5.00	0	0	0
1	0.015	4.985	99.70	3.32×10^5
2	0.013	4.987	99.74	3.84×10^5
3	0.0055	4.994	99.88	9.08×10^5
5	0.0039	4.996	99.92	1.28×10^6
10	0.0053	4.995	99.90	9.42×10^5
20	0.0058	4.994	99.88	8.61×10^5
30	0.0050	4.995	99.90	9.99×10^5
60	0.0071	4.993	99.86	7.03×10^5
90	0.0067	4.993	99.86	7.45×10^5
120	0.011	4.989	99.78	4.54×10^5
180	0.017	4.983	99.66	2.93×10^5
300	0.026	4.974	99.48	1.91×10^5
360	0.033	4.967	99.34	1.51×10^5
480	0.037	4.963	99.26	1.34×10^5
600	0.033	4.967	99.34	1.51×10^5

Table S3. The Sr^{2+} adsorption kinetics results of **Na-Dy** (V/m = 1000 mL/g; at room temperature (RT)).

Time (minute)	C_t (mg/L)	q (mg/g)	R^{Sr} (%)	K_d^{Sr} (mL/g)
0	5.28	0	0	0
1	0.0215	5.259	99.59	2.45×10^5
2	0.0125	5.268	99.76	4.21×10^5
3	0.0073	5.273	99.86	7.22×10^5
5	0.0044	5.276	99.92	1.20×10^6
10	0.0035	5.277	99.93	1.53×10^6
20	0.0042	5.276	99.92	1.26×10^6
30	0.0043	5.276	99.92	1.23×10^6
60	0.0043	5.276	99.92	1.23×10^6
90	0.0145	5.266	99.73	3.63×10^5
120	0.0210	5.259	99.60	2.50×10^5

180	0.0270	5.253	99.49	1.95×10^5
300	0.0300	5.250	99.43	1.75×10^5
360	0.0300	5.250	99.43	1.75×10^5
480	0.0310	5.249	99.41	1.69×10^5
600	0.0330	5.247	99.38	1.59×10^5

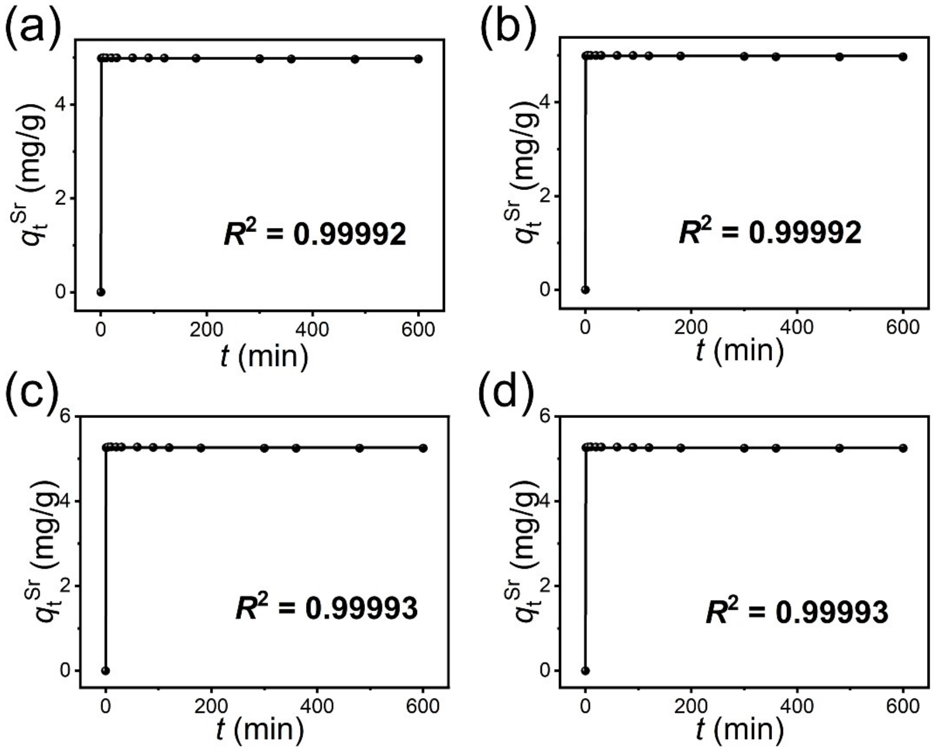

Figure S3. The fitting results with the pseudo-first-order kinetic model for the Sr^{2+} ions removal kinetics of **K-Dy** (a) and **Na-Dy** (c). The fitting results with the pseudo-second-order kinetic model for the Sr^{2+} ions removal kinetics of **K-Dy** (b) and **Na-Dy** (d).

6. Adsorption isotherms

Table S4. Isothermal adsorption experimental results of Sr^{2+} capture by **K-Dy** (V/m = 1000 mL/g; 8 h contact time; at RT).

C_0 (mg/L)	C_e (mg/L)	q (mg/g)
5.33	0.0078	5.32
11.00	0.033	10.97
51.65	2.93	48.72
104.30	44.34	59.96
203.37	135.61	67.76
325.75	249.55	76.20
403.47	335.07	68.40
834.58	752.73	81.85

Table S5. Isothermal adsorption experimental results of Sr^{2+} capture by **Na-Dy** (V/m = 1000 mL/g; 8 h contact time; at RT).

C_0 (mg/L)	C_e (mg/L)	q (mg/g)
5.20	0.22	4.98
11.30	0.11	11.19
51.82	0.47	51.35
103.74	29.04	74.70
321.46	233.82	87.64
413.38	329.09	84.29
620.75	543.50	77.25
815.50	739.25	76.25

Table S6. Isotherm fitting parameters for Sr^{2+} capture by **K-Dy** (V/m = 1000 mL/g; 8 h contact time; at RT).

	Langmuir	Freundlich	Langemiur-Freundlich
R^2	0.9406	0.9334	0.9785
q (mg/g)	71.72 ± 3.59	-	83.04 ± 8.48
b	0.7123	-	0.4554
n	-	6.6596	2.4226
k	-	31.4769	-

Table S7. Isotherm fitting parameters for Sr^{2+} capture by **Na-Dy** (V/m = 1000 mL/g; 8 h contact time; at RT).

	Langmuir	Freundlich	Langemiur-Freundlich
R^2	0.9159	0.3242	0.9676
q (mg/g)	80.96 ± 4.67	-	79.93 ± 3.14
b	1.7295	-	2.4526
n	-	42.6736	0.2672
k	-	70.2673	-

7. The effect of pH and irradiation on Sr^{2+} adsorption

Table S8. The pH effect adsorption results of **K-Dy** for Sr^{2+} removal (V/m = 1000 mL/g; at RT; 8 h contact time).

Initial pH	C_0^{Sr} (mg/L)	C_e^{Sr} (mg/L)	q (mg/g)	R^{Sr} (%)	K_d^{Sr} (mL/g)	Leaching percentage of Dy (%)
1.99	5.60	5.53	0.070	1.25	12.66	44.64
2.97	5.16	0.11	5.05	97.87	4.59×10^4	0.40
3.94	5.14	0.015	5.12	99.61	3.41×10^5	0.41
4.93	5.03	0.015	5.02	99.80	3.35×10^5	0.46
5.90	5.08	0.020	5.06	99.61	2.53×10^5	0.42
7.20	5.02	0.024	5.00	99.60	2.08×10^5	0.69
8.00	4.92	0.012	4.91	99.80	4.09×10^5	0.36
9.00	4.90	0.027	4.87	99.39	1.80×10^5	0.24
10.00	4.91	0.012	4.90	99.80	4.08×10^5	0.34
10.91	4.94	0.018	4.92	99.60	2.73×10^5	0.56
11.84	4.81	0.060	4.75	98.75	7.92×10^4	0.090

Table S9. The results of Sr^{2+} adsorption for **K-Dy** before and after irradiations (V = 10 mL, m = 10 mg, V/m = 1000 mL/g; 8 h contact time; at RT).

		C_0^{Sr} (mg/L)	C_e^{Sr} (mg/L)	q^{Sr} (mg/g)	K_d^{Sr} (mL/g)	R^{Sr} (%)
K-Dy	Pristine	4.80	0.0094	4.7906	5.10×10^5	99.80
	100 kGy γ	4.80	0.0099	4.7901	4.84×10^5	99.79
	200 kGy γ	4.80	0.017	4.783	2.81×10^5	99.65

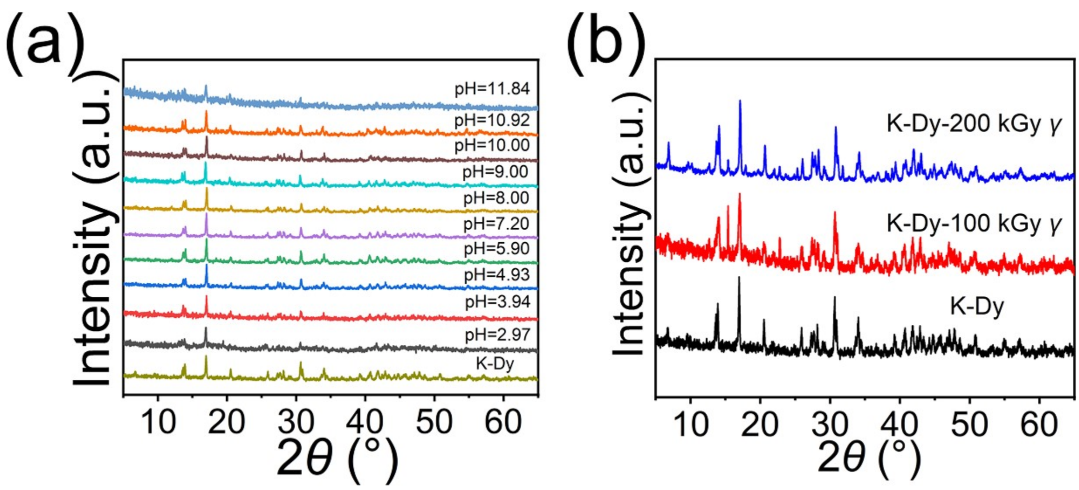

Figure S4. (a) PXRD patterns of **K-Dy** synthesized and its corresponding samples in Sr^{2+} solutions with different pH values. (b) PXRD patterns of the pristine and γ (100 and 200 kGy) irradiated samples of **K-Dy**.

8. Adsorption and desorption

Table S10. The adsorption and desorption results for **K-Dy** at each cycle.

Number of cycles	Adsorption					Desorption			
	m (mg)	V (mL)	C_0^{Sr} (mg/L)	C_e^{Sr} (mg/L)	R^{Sr} (%)	m_1 (mg)	V_1 (mL)	C_e^{Sr} (mg/L)	E^{Sr} (%)
1	200	200	5.60	0.07	98.80	160	160	4.71	85.14
2	130	130	5.68	0.02	99.60	100	100	5.54	97.96
3	70	70	5.74	0.03	99.50	40	40	5.31	93.17

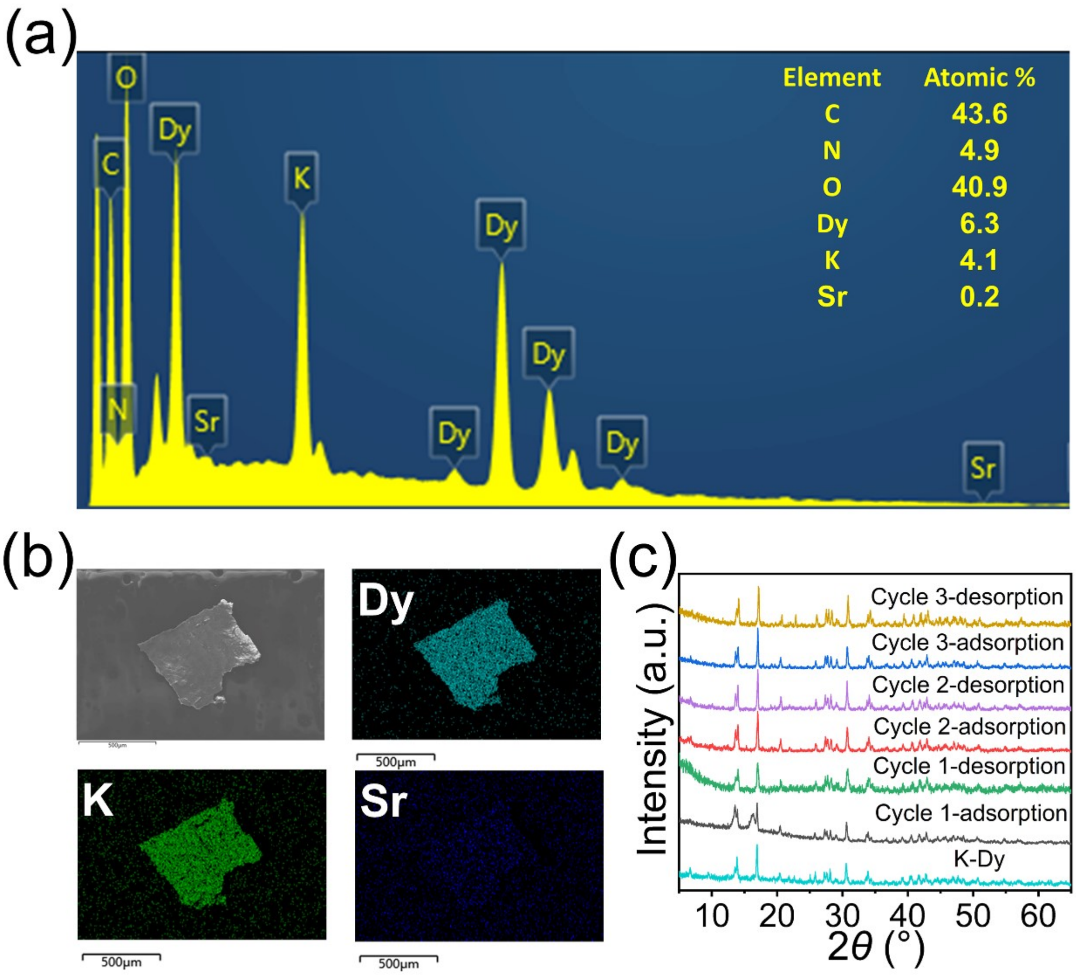

Figure S5. (a) EDS analysis results and (b) elemental distribution mappings of **K-Dy** after desorption. (c) PXRD patterns of **K-Dy** after adsorption and desorption.

9. Competitive adsorption

Table S11. The Sr^{2+} and Na^+ adsorption results of **K-Dy** under different Na/Sr molar ratios (V/m = 1000 mL/g; at RT; 8 h contact time).

Molar Ratio (Na/Sr)	Sr^{2+}	C_0 (mg/L)	$\pm C_0$ (mg/L)	C_e (mg/L)	$\pm C_e$ (mg/L)	K_d (mL/g)	$\pm K_d$ (mL/g)	R (%)	$\pm R$ (%)	
9		5.69	0.0566	0.01	0.0008	1.01×10^6	140232.94	99.90	0.0139	
44		5.21	0.0636	0.02	0.0028	3.10×10^5	55452.06	99.67	0.0583	
92		5.26	0.0424	0.03	0.0000	1.63×10^5	1325.83	99.39	0.0049	
476		5.22	0.0849	0.30	0.0007	1.63×10^4	320.84	94.20	0.1078	
	Na^+	C_0 (mg/L)	$\pm C_0$ (mg/L)	C_e (mg/L)	$\pm C_e$ (mg/L)	K_d (mL/g)	$\pm K_d$ (mL/g)	R (%)	$\pm R$ (%)	$SF_{Sr/Na}$
		13.46	0.3606	9.85	0.1697	3.66×10^2	13.08	26.78	0.7011	2754.16
		60.01	0.5091	52.73	0.0283	1.38×10^2	9.04	12.13	0.6984	2243.89
		126.75	1.2021	114.25	1.0607	1.09×10^2	0.22	9.86	0.0180	1493.26
		651.65	7.4246	618.70	3.2527	5.33×10^1	17.54	5.05	1.5810	304.98

Table S12. The Sr^{2+} and Cs^+ adsorption results of **K-Dy** under different Cs/Sr molar ratios (V/m = 1000 mL/g; at RT; 8 h contact time).

Molar Ratio (Cs/Sr)	Sr^{2+}	C_0 (mg/L)	$\pm C_0$ (mg/L)	C_e (mg/L)	$\pm C_e$ (mg/L)	K_d (mL/g)	$\pm K_d$ (mL/g)	R (%)	$\pm R$ (%)	
10		5.05	0.0707	0.2650	0.0071	1.81×10^4	241.75	94.75	0.0666	
100		5.04	0.0566	0.0315	0.0078	1.64×10^5	38898.22	99.38	0.1473	
513		4.97	0.0071	0.1445	0.0106	3.35×10^4	2577.97	97.09	0.2178	
970		5.21	0.0566	0.4395	0.0035	1.09×10^4	33.35	91.56	0.0237	
	Cs^+	C_0 (mg/L)	$\pm C_0$ (mg/L)	C_e (mg/L)	$\pm C_e$ (mg/L)	K_d (mL/g)	$\pm K_d$ (mL/g)	R (%)	$\pm R$ (%)	$SF_{Sr/Cs}$
		76.10	0.2828	55.00	0.0000	3.84×10^2	5.14	27.73	0.2686	47.08
		765.00	2.8284	658.00	1.4142	1.63×10^2	6.80	13.99	0.5029	1007.26
		3865.00	7.0711	3850.00	7.0711	3.90×10^0	0.01	0.39	0.0007	8586.63
		7660.00	56.5685	7540.00	28.2843	1.59×10^1	3.69	1.57	0.3577	682.31

Table S13. The Sr^{2+} and Mg^{2+} adsorption results of **K-Dy** under different Mg/Sr molar ratios (V/m = 1000 mL/g; at RT; 8 h contact time).

Molar Ratio (Mg/Sr)	Sr^{2+}	C_0 (mg/L)	± C_0 (mg/L)	C_e (mg/L)	± C_e (mg/L)	K_d (mL/g)	± K_d (mL/g)	R (%)	± R (%)
1		5.14	0.2121	0.07	0.0000	7.57×10^4	3166.15	98.70	0.0538
9		5.12	0.0283	0.12	0.0014	4.17×10^4	738.59	97.66	0.0406
44		5.17	0.0354	1.60	0.0071	2.24×10^3	7.81	69.12	0.0745
91		5.38	0.0424	2.60	0.0354	1.07×10^3	11.90	51.77	0.2768
	Mg^{2+}	C_0 (mg/L)	± C_0 (mg/L)	C_e (mg/L)	± C_e (mg/L)	K_d (mL/g)	± K_d (mL/g)	R (%)	± R (%)
		1.91	0.2333	0.12	0.0113	1.48×10^4	3375.22	93.51	1.3888
		12.62	0.1344	1.02	0.0141	1.14×10^4	303.22	91.91	0.1982
		63.59	0.5374	47.68	0.1273	3.34×10^2	14.83	25.02	0.8338
		135.35	1.0607	115.95	0.9192	1.67×10^2	0.11	14.33	0.0078

Table S14. The Sr^{2+} and Ca^{2+} adsorption results of **K-Dy** under different Ca/Sr molar ratios (V/m = 1000 mL/g; at RT; 8 h contact time).

Molar Ratio (Ca/Sr)	Sr^{2+}	C_0 (mg/L)	± C_0 (mg/L)	C_e (mg/L)	± C_e (mg/L)	K_d (mL/g)	± K_d (mL/g)	R (%)	± R (%)
1		5.13	0.1273	0.08	0.0092	6.02×10^4	8158.92	98.35	0.2201
8		5.45	0.0212	0.12	0.0028	4.29×10^4	1172.99	97.72	0.0608
41		5.43	0.0778	2.91	0.0354	8.67×10^2	4.05	46.45	0.1161
81		5.48	0.0495	3.90	0.0141	4.04×10^2	17.78	28.76	0.9023
	Ca^{2+}	C_0 (mg/L)	± C_0 (mg/L)	C_e (mg/L)	± C_e (mg/L)	K_d (mL/g)	± K_d (mL/g)	R (%)	± R (%)
		3.13	0.2475	0.22	0.0481	1.35×10^4	4263.68	92.81	2.1079
		20.35	0.0849	1.08	0.0636	1.80×10^4	1043.56	94.72	0.2907
		101.35	0.4950	76.49	0.7212	3.25×10^2	6.02	24.53	0.3431
		203.90	0.4243	173.15	0.6364	1.78×10^2	6.78	15.08	0.4888

Table S15. The Sr^{2+} adsorption results of **K-Dy** in the presence of Sr^{2+}, Na^+, Cs^+, Mg^{2+}, Ca^{2+} ions with the same mass concentration (V/m = 1000 mL/g; at RT; 8 h contact time).

Ion	C_0 (mg/L)	± C_0 (mg/L)	C_e (mg/L)	± C_e (mg/L)	K_d (mL/g)	± K_d (mL/g)	R (%)	± R (%)
Sr^{2+}	5.91	0.1231	0.09	0.0236	6.50×10^4	15576.91	98.44	0.3676

Cs^+	4.91	0.0000	3.35	0.0016	4.66×10^2	0.72	31.78	0.0336
Na^+	4.33	0.0002	2.86	0.1344	5.13×10^2	70.97	33.82	3.1044
Mg^{2+}	6.10	0.0830	1.21	0.0156	4.04×10^3	133.41	80.14	0.5259
Ca^{2+}	14.53	0.3052	10.09	0.2620	4.39×10^2	7.14	30.53	0.3445

Table S16. The results of Sr^{2+} ions removal efficiency by **K-Dy** in actual water samples contaminated with Sr^{2+} ions (V/m = 1000 mL/g, at RT; 8 h contact time).

Water	C_0 (mg/L)	$\pm C_0$ (mg/L)	C_e (mg/L)	$\pm C_e$ (mg/L)	K_d (mL/g)	$\pm K_d$ (mL/g)	R (%)	$\pm R$ (%)
Ultrapure water	2.20	0.0212	0.01	0.0001	3.37×10^5	9010.69	99.70	0.0079
River water	5.08	0.0171	0.05	0.0014	9.63×10^4	2928.88	98.97	0.0310
Tap water	5.13	0.0629	0.10	0.0239	5.36×10^4	12842.19	98.12	0.4429

10. Adsorption Mechanism

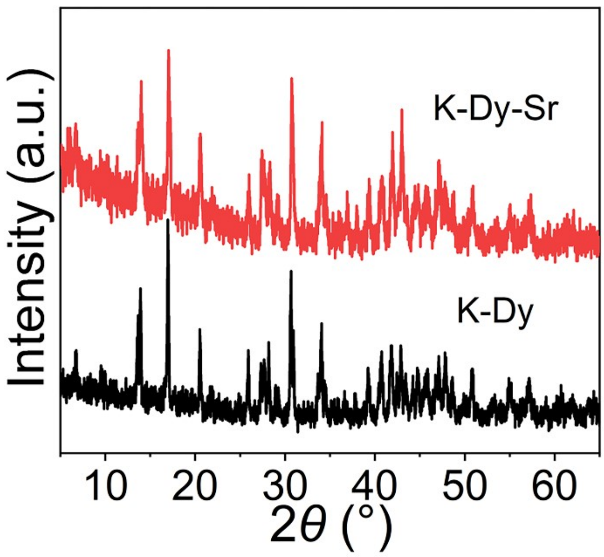

Figure S6. PXRD patterns for the pristine K-Dy and K-Dy-Sr.

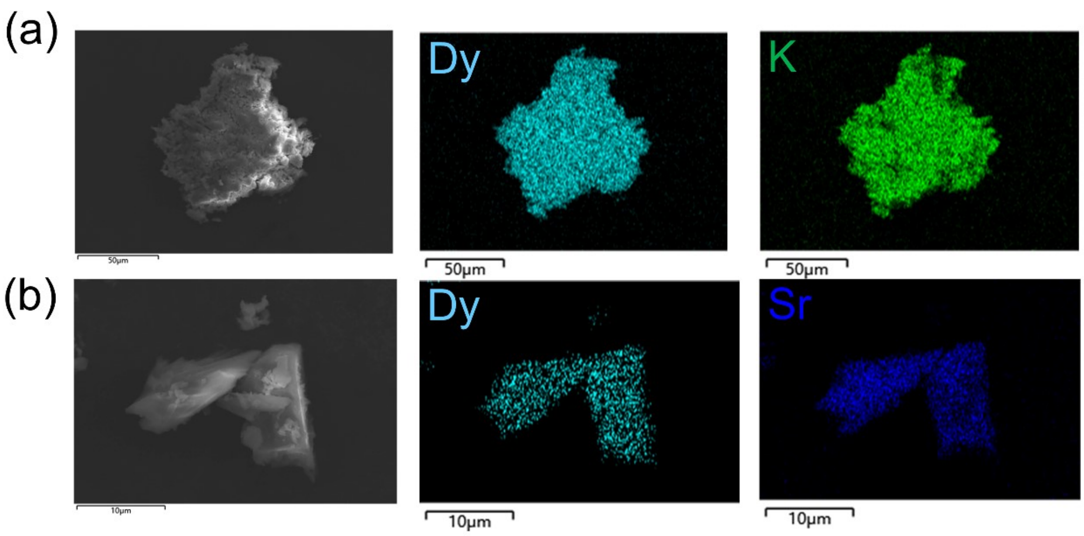

Figure S7. The scanning electron microscopy images and the elemental distribution mappings of **K-Dy** (a) and **K-Dy-Sr** (b).

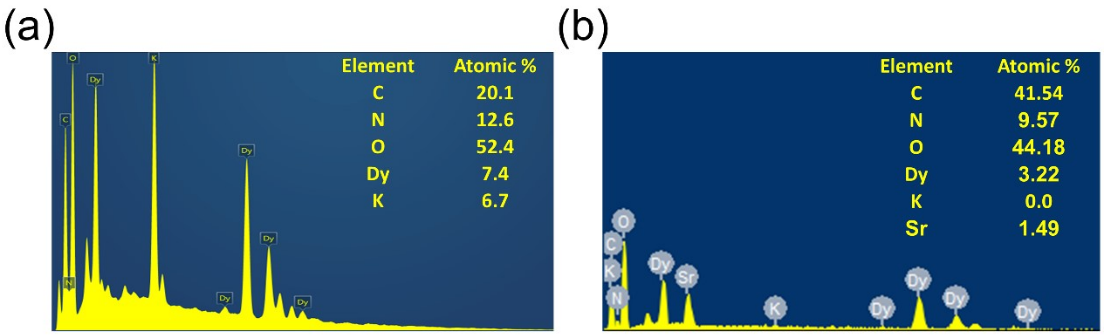

Figure S8. EDS analysis results of **K-Dy** (a) and **K-Dy-Sr** (b).