*Supporting information for*

# HKUST-1 Water-Resistant Functionalized with Polydimethylsiloxane for Rubidium Ion Efficient Capture

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**Table S1.** The structural information of MOFs prepared in this work.

| Samples | $S_{BET}$ ($m^2/g$) | $V_{total}$ (mL/g) | $V_{meso}$ (mL/g) | $V_{mic}$ (mL/g) | Average pore diameter (nm) |
|---|---|---|---|---|---|
| HKUST-1 | 1242.76 | 0.58 | 0.10 | 0.48 | 2.15 |
| HKUST-1(R1) | 448.17 | 0.22 | 0.05 | 0.17 | 0.95 |
| HKUST-1(R2) | 291.20 | 0.29 | 0.09 | 0.20 | 0.35 |
| PDMS(0.5)@ HKUST-1 | 1156.70 | 0.51 | 0.07 | 0.44 | 1.82 |
| PDMS(1.0)@ HKUST-1 | 1103.70 | 0.54 | 0.15 | 0.39 | 1.96 |
| PDMS(2.0)@ HKUST-1 | 1102.64 | 0.46 | 0.05 | 0.41 | 1.74 |
| PDMS(2.0)@ HKUST-1(R1) | 1093.58 | 0.42 | 0.04 | 0.38 | 1.69 |
| PDMS(2.0)@ HKUST-1(R5) | 1082.42 | 0.41 | 0.04 | 0.37 | 1.65 |
| PDMS(3.0)@ HKUST-1 | 1100.90 | 0.46 | 0.04 | 0.42 | 1.72 |

**Table S2.** Element composition of SEM-EDS analysis for HKUST-1 and PDMS(2.0)@HKUST-1.

| Sample | Element content, % | | | | |
|---|---|---|---|---|---|
| | Si | Cu | C | O | Total |
| HKUST-1 | 0 | 13.49 | 55.28 | 31.23 | 100 |
| PDMS(2.0)@HKUST-1 | 1.71 | 7.42 | 57.39 | 33.48 | 100 |

**Table S3** Comparison of adsorption capability and reusability of $Rb^+$ on some MOFs materials.

| Adsorbent | Adsorption capacities (mg/g) | Reusability (mg/g) | Reference |
|---|---|---|---|
| PMA@ HKUST-1 | 93 | 45 (twice) | (14) |
| PH@MIL-101(Cr) | 89 | 80 (5 times) | (13) |
| MIL-101(Cr) | 73 | 66 (5 times) | (13) |
| MIL-53(Al) | 51 | 25 (twice) | (14) |
| HS-$Fe_3O_4$@MIL-53(Al) | 86 | 65 (twice) | (9) |
| HKUST-1 | 82 | 8 (3 times) | This work |
| PDMS@HKUST-1 | 82 | 82 (5 times) | This work |

**Table S4.** Adsorption isotherm models used in this study and their linear forms.

| Isotherm | Nonlinear form | Linear form | Plot |
|---|---|---|---|
| Langmuir-I | $q_e = \frac{K_L C_e}{1 + K_L C_e}$ | $\frac{C_e}{q_e} = \frac{1}{q_L \cdot K_L} + (\frac{1}{q_L}) \cdot C_e$ | $\frac{C_e}{q_e}$ versus $C_e$ |
| Freundlich | $q_e = K_f C_e^{\frac{1}{n}}$ | $\ln q_e = \ln K_f + (\frac{1}{n}) \cdot \ln C_e$ | $\ln q_e$ versus $\ln C_e$ |
| Temkin | $e^{qe} = (K_T C_e)^{\frac{RT}{b_T}}$ | $q_e = \frac{RT}{b_T} \ln K_T + \frac{RT}{b_T} \ln C_e$ | $q_e$ versus $\ln C_e$ |
| D–R | $q_e = q_s e^{(-K_D \varepsilon^2)}$ | $\ln q_e = \ln q_s - K_D \varepsilon^2$ | $\ln q_e$ versus $\varepsilon^2$ |

Where $q_e$ is the maximum capacity of adsorption in mg/g; $K_L$ is a constant related to the affinity of the binding sites in L/mg; '$K_f$' and '$n$' are the measures of adsorption capacity and intensity of adsorption; $R$ is the universal gas constant; $b_T$ is related to the heat of adsorption in kJ/mol. T is the absolute temperature in K; $R$ is the universal gas constant; $K_T$ is the Temkin constant about the capacity of adsorption in L/g; $q_s$ is the D-R isotherm constant in mg/g; $K_D$ stands for the constant that is relevant with the adsorption energy in $mol^2/kJ^2$; $\varepsilon$ represents the Polanyi potential constant in kJ/mol;

**Table S5.** Constants and correlation coefficients of different adsorption models for HKUST-1 before and after coated with PDMS.

| Samples | Langmuir | | | Freundlich | | | Temkin | | | D-R | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $q_m$ (mg/g) | $K_L$ ($L$/mg) | $R^2$ | $K_f$ ($L$/g) | $n$ | $R^2$ | $b_T$ (kJ/mol) | $K_T$ ($L$/g) | $R^2$ | $q_s$ (mg/g) | $K_D$ ($mol^2/kJ^2$) | $R^2$ |
| HKUST-1 | 83.76 | 0.0052 | 0.2529 | 1.3843 | 1.0305 | 0.9942 | 78.39 | 0.1372 | 0.8631 | 1.46E-05 | 51.05 | 0.6560 |
| HKUST-1R1 | 42.24 | 0.0029 | 0.2067 | 0.2896 | 0.8799 | 0.9844 | 146.44 | 0.0986 | 0.9051 | 3.35E-05 | 27.12 | 0.8017 |
| HKUST-1R2 | 7.74 | 0.0204 | 0.4997 | 0.2041 | 1.1654 | 0.7047 | 1271.16 | 0.2501 | 0.5468 | 4.29E-05 | 6.03 | 0.8892 |
| PDMS(0.5)@HKUST-1 | 83.45 | 0.0045 | 0.2107 | 1.3233 | 1.0063 | 0.9931 | 76.38 | 0.1406 | 0.8804 | 1.46E-05 | 52.68 | 0.6686 |
| PDMS(1.0)@HKUST-1 | 83.18 | 0.0017 | 0.2042 | 1.3085 | 1.0021 | 0.9924 | 76.51 | 0.1401 | 0.8759 | 1.47E-05 | 52.67 | 0.6687 |
| PDMS(2.0)@HKUST-1 | 82.18 | 0.0054 | 0.35 | 2.3858 | 1.1880 | 0.9901 | 84.67 | 0.1718 | 0.8451 | 1.01E-05 | 52.45 | 0.6221 |
| PDMS(3.0)@HKUST-1 | 82.76 | 0.0066 | 0.2522 | 0.8939 | 0.9415 | 0.9909 | 80.43 | 0.1252 | 0.8873 | 2.16E-05 | 50.85 | 0.7864 |
| PDMS(2.0)@HKUST-1R1 | 82.11 | 0.0026 | 0.2561 | 1.6525 | 1.0659 | 0.9887 | 78.89 | 0.1491 | 0.8978 | 1.55E-05 | 54.79 | 0.7476 |
| PDMS(2.0)@HKUST-1R5 | 51.90 | 0.0021 | 0.2020 | 0.6179 | 0.9562 | 0.9867 | 113.16 | 0.1157 | 0.9374 | 2.55E-05 | 36.76 | 0.7713 |

**Table S6.** Kinetic calculation equations.

| Name | equations |
|---|---|
| Pseudo-first order model | $\ln(q_e - q_t) = \ln(q_e) - K_1 t$ |
| Pseudo-second order model | $\frac{t}{q_t} = \frac{1}{K_2 q_e} + \frac{t}{q_e}$ |
| Intra-particle diffusion model | $q_t = K_3 t^{1/2}$ |
| Normalized standard deviation | $\Delta q(\%) = \frac{(q_{e,\exp} - q_{e,cal})}{q_{e,\exp}} \times 100\%$ |

Where $q_e$ and $q_t$ (mg/g) are the uptakes of thiophene at equilibrium and at time $t$ (min), respectively, $K_1$ (1/min) is the adsorption rate constant, $K_2$ (g/mg.min) is the rate constant for the second-order equation, and $K_3$ (mg/g.min$^{1/2}$) is the intra-particle diffusion rate constant.

Where $q_{e,exp}$ and $q_{e,cal}$ are the experimental and calculation uptakes of CR, respectively.

**Table S7.** Kinetic parameters for Rb(I) adsorption on HKUST-1 before and after coated with PDMS.

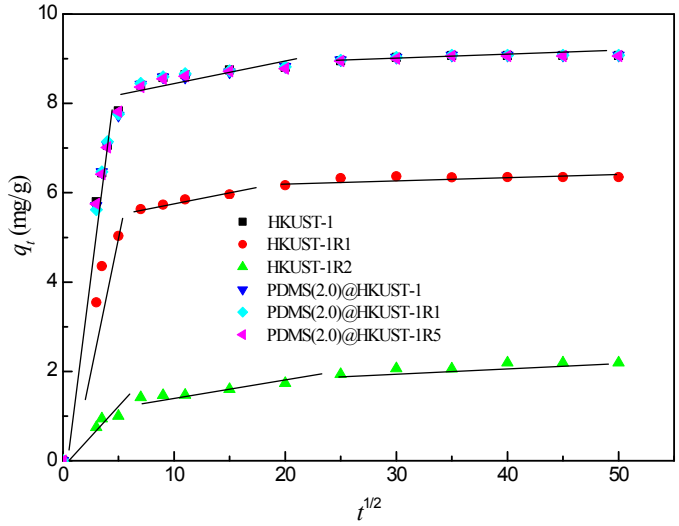
| Sample | Pseudo-first-order rate equation | | | | | | Pseudo-second-order rate equation | | | | | Intra-particle diffusion model | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $q_{e,exp}$ (mg/g) | $q_{e,cal}$ (mg/g) | $K_1$ (1/min) | $R^2$ | $\Delta q$ (mg/g) | $\Delta q$ (%) | $q_{e,cal}$ (mg/g) | $K_2$ (g/mg·min) | $R^2$ | $\Delta q$ (mg/g) | $\Delta q$ (%) | $C$ (mg/g) | $K_3$ (mg/g·min$^{1/2}$) | $R^2$ |
| HKUST-1 | 83 | 14.401 | -0.09 | 0.664 | 68.59 | 82.65 | 84.10 | 0.01 | 0.999 | -1.10 | -1.33 | 64.85 | 2.49 | 0.632 |
| HKUST-1R1 | 41 | 6.615 | -0.086 | 0.529 | 34.38 | 83.87 | 41.78 | 0.01 | 0.998 | -0.789 | -1.92 | 27.38 | 1.87 | 0.627 |
| HKUST-1R2 | 5 | 4.499 | -0.053 | 0.909 | 0.500 | 10.01 | 6.37 | 0.008 | 0.966 | -1.37 | -27.4 | 0.36 | 0.59 | 0.868 |
| PDMS(2.0)@HKUST-1 | 83 | 18.445 | -0.12 | 0.677 | 64.55 | 77.78 | 84.32 | 0.01 | 0.999 | -1.32 | -1.59 | 64.03 | 0.63 | 0.616 |
| PDMS(2.0)@HKUST-1R1 | 83 | 16.414 | -0.115 | 0.608 | 66.59 | 80.22 | 84.25 | 0.01 | 0.999 | -1.246 | -1.50 | 64.73 | 2.53 | 0.602 |
| PDMS(2.0)@HKUST-1R5 | 46 | 8.485 | -0.06 | 0.928 | 37.52 | 81.55 | 46.38 | 0.015 | 0.999 | -0.38 | -0.83 | 35.50 | 1.41 | 0.599 |

**Figure S captions:**

**Fig. S1** Weber–Morris intra-particle diffusion plots for the adsorption of Rb(I) on HKUST-1 and PDMS(2.0)@HKUST-1 before and after recycle use.

**Fig. S2** Effect of pH on the zeta potential of HKUST-1.

**Fig. S3** Effect of pH on the Rb(I) uptake capacity of HKUST-1.

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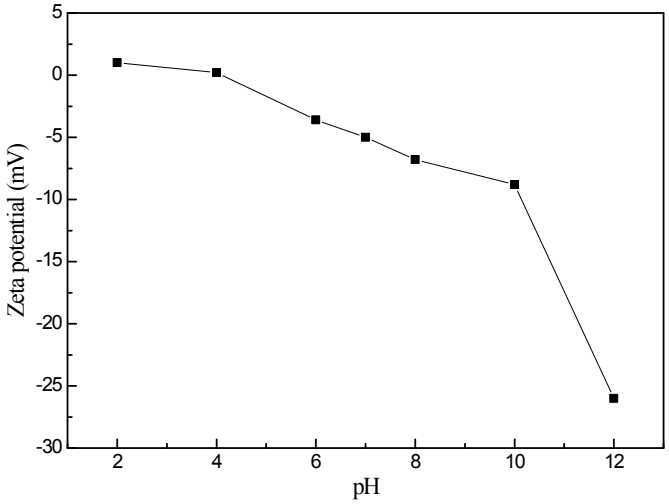
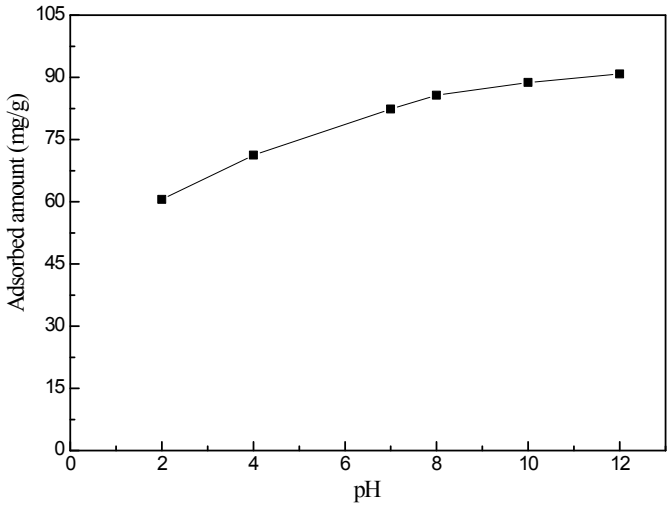



**Fig. S2.** Effect of pH on the zeta potential of HKUST-1.

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