Electronic Supplementary Material (ESI) for RSC Advances.

The calculation method for SNE

(1) Select one isotherm and one error function (for example, the *ERRSQ* error function) and get the *solver add-in* output to determine the isotherm parameters in a way that minimizes the applied error function (in this case, *ERRSQ*). (If the applied error function is the coefficient of determination, the *solver add-in* must be adjusted on maximizing.)

(2) Determine the values of other error functions based on isotherm parameters obtained from step (1).

(3) Perform the above steps exactly for all other error functions.

(4) Select the maximum output of each error function from all sets. In order to calculate the normalized error, the value of other sets should be divided into the maximum value. This should be done for all error functions.

(5) Calculate the summation of all of these normalized errors for each parameter.

Table S1: Lists of error functions

Error function	Abbreviation	Definition/expression
The coefficient of determination	R^2	$R^2 = \frac{\sum\left(q_{e,meas} - \bar{q}_{e,calc}\right)^2}{\sum\left(q_{e,meas} - \bar{q}_{e,calc}\right)^2 + \sum\left(q_{e,meas} - q_{e,calc}\right)^2}$
Nonlinear chi-square test	χ^2	$\chi^2 = \sum_{i=1}^{n} \frac{\left(q_{e,meas} - q_{e,calc}\right)^2}{q_{e,meas}}$
Residual root mean square error	*RMSE*	$\mathrm{RMSE} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}\left(q_{e,meas} - q_{e,calc}\right)^2}$
Average relative error	*ARE*	$ARE = \frac{100}{n}\sum_{i=1}^{n}\left\lvert\frac{q_{e,meas} - q_{e,calc}}{q_{e,meas}}\right\rvert$
Standard deviation of relative errors	S_{RE}	$S_{RE} = \sqrt{\frac{\sum_{i=1}^{n}\left[\left(q_{e,meas} - q_{e,calc}\right) - ARE\right]^2}{n-1}}$
Marquardt's percent standard deviation	*MPSD*	$\mathrm{MPSD} = 100\sqrt{\frac{1}{n-p}\sum_{i=1}^{n}\left(\frac{q_{e,meas} - q_{e,calc}}{q_{e,meas}}\right)^2}$
Sum squares errors	*ERRSQ*	$\mathrm{ERRSQ} = \sum_{i=1}^{n}\left(q_{e,meas} - q_{e,calc}\right)^2$

q_{meas}: Measured ion concentration; q_{calc}: calculated ion concentration with models; n: the number of experimental data points; p: the number of parameters in each isotherm model.

Table S2. Mathematical equations of the single-component isotherm models employed [33]

Isotherm	Non-linear equation	Linear equation
Freundlich	$q_e = K_f C_e^{1/n}$	$\ln(q_e) = \ln(\mathrm{K}_f) + \frac{1}{n}\ln(\mathrm{C}_e)$
Langmuir	$q_e = \frac{q_m K_a C_e}{1 + K_a C_e}$	$\frac{C_e}{q_e} = \frac{1}{q_m} C_e + \frac{1}{K_a q_m}$
Redlich–Peterson	$q_e = \frac{A C_e}{1 + B C_e^{\ m}}$	$\ln(A\frac{\mathrm{C}_e}{q_e} - 1) = m\ln(\mathrm{C}_e) + \ln(\mathrm{B})$

[a] K_f: Freundlich isotherm constant [(mg/g)(L/mg)$^{1/n}$]; [b] n: Freundlich exponent (dimensionless)
[c] q_m: Langmuir monolayer adsorption capacity (mg/g); [d] K_a: Langmuir isotherm constant (L/mg)
[e] A: Redlich–Peterson isotherm constant (L/g); [f] B: Redlich Peterson isotherm constant (L/mg)$^{1/m}$
[g] m: Redlich-Peterson constant.

Table S3. The isotherm parameters and error deviation data for the adsorption of Pb(II) onto $ZnCl_2$-MCM-41 obtained by non-linear regression method (T=20 °C, pH=7, sorbent dosage=0.333 g L^{-1}, 60 min, 300 rpm)

Freundlich (two parameter isotherm)							
	R^2	χ^2	*RMSE*	*ARE*	S_{RE}	*MPSD*	*ERRSQ*
K_f	56.7	55.6	56.4	42.6	50.4	43.4	56.5
$1/n$	0.576	0.626	0.577	0.663	0.624	0.697	0.577
R^2	0.991313	0.986864	0.991313	0.980046	0.985037	0.961906	0.991313
χ^2	22.45112448	11.8379	15.8801	18.6419	15.1521	19.2883	15.72590
RMSE	23.1949	28.5768	23.1913	35.4180	30.5727	49.2948	23.1913
ARE	22.5491	16.0817	22.3045	10.7155	14.6455	10.9127	22.3049
S_{RE}	35.8897	31.3583	35.4203	27.3824	24.2253	45.0168	35.4207
MPSD	43.3860	26.1996	42.9553	17.2372	23.3644	15.4520	42.9560
ERRSQ	1614.01	2449.9083	1613.51	3763.33	2804.05	7289.94	1613.51
SNE	5.4891	4.4522	5.1965	4.5344	4.3995	5.66957	5.15833
Langmuir (two parameter isotherm)							
	R^2	χ^2	*RMSE*	*ARE*	S_{RE}	*MPSD*	*ERRSQ*
q_m	506.5	479.1	506.6	440.4	516.5	426.8	506.6
K_a	0.142	0.155	0.142	0.171	0.130	0.176	0.142
R^2	0.999494	0.999027	0.999494	0.996972	0.997694	0.995741	0.999494
χ^2	1.4282	1.0645	1.4307	1.7224	4.1567	2.1284	1.4307

RMSE	5.5688	7.7290	5.5688	13.6498	11.9210	16.1978	5.5688
ARE	5.9452	4.5185	5.9513	4.1043	10.0124	4.3710	5.9513
S_{RE}	6.3097	8.4609	6.2984	12.7020	2.4732	14.5385	6.2984
MPSD	10.9172	7.9592	10.9271	6.3112	16.3789	6.2407	10.9271
ERRSQ	93.0358	9.7480	93.0346	558.9575	426.3332	787.1149	93.0346
SNE	3.4999	3.2643	3.5009	4.6336	5.4459	5.3258	3.5009

Redlich-Peterson (three parameter isotherm)

	R^2	χ^2	*RMSE*	*ARE*	S_{RE}	*MPSD*	*ERRSQ*
A	75.84	79.93	75.84	75.83	68.30	84.76	75.84
B	0.2802	0.3098	0.2802	0.2802	0.2452	0.3546	0.2802
m	0.837	0.815	0.837	0.837	0.861	0.780	0.837
R^2	0.999981	0.999969	0.999981	0.999981	0.999776	0.999855	0.999981
χ^2	0.0962	0.0744	0.0962	0.0962	0.4571	0.1245	0.0962
RMSE	1.0575	1.3712	1.0575	1.0579	3.7023	2.9823	1.0575
ARE	1.3131	1.3598	1.3130	1.3117	3.3594	1.3884	1.3130
S_{RE}	1.5299	1.9357	1.5293	1.5152	0.8018	3.0014	1.5293
MPSD	3.9737	2.9856	3.9740	3.9752	7.5103	2.5850	3.9740

Table S4

Comparison of monolayer maximum adsorption capacities (q_{max}) of some adsorbents for Pb(II) removal from aqueous solution

Sorbent	Initial concentration (mg/L)	Amount of adsorbent (g/L)	Adsorption capacity (mg/g)
Polyvinyltetrazole-grafted resin [1]	103-1656	1.0	314.9
Acrylonitrile–Butadiene–Styrene [2]	20-300	4.0	56.5
Nanostructured BiOBr [3]	2-40	0.5	6.5
Thiol grafted on silica gel [4]	207-1656	2.5	497.1
Fe_3O_4 nanocapsules [5]	0.1-50	0.5	79.0
Amine grafted mesoporous silica embedded with nano-magnetite [6]	10-20	0.667	222.4
Amino siloxane oligomer-linked graphene oxide [7]	10-400	1.0	312.5
$ZnCl_2$-MCM-41 (this work)	2-200	0.33	479.0

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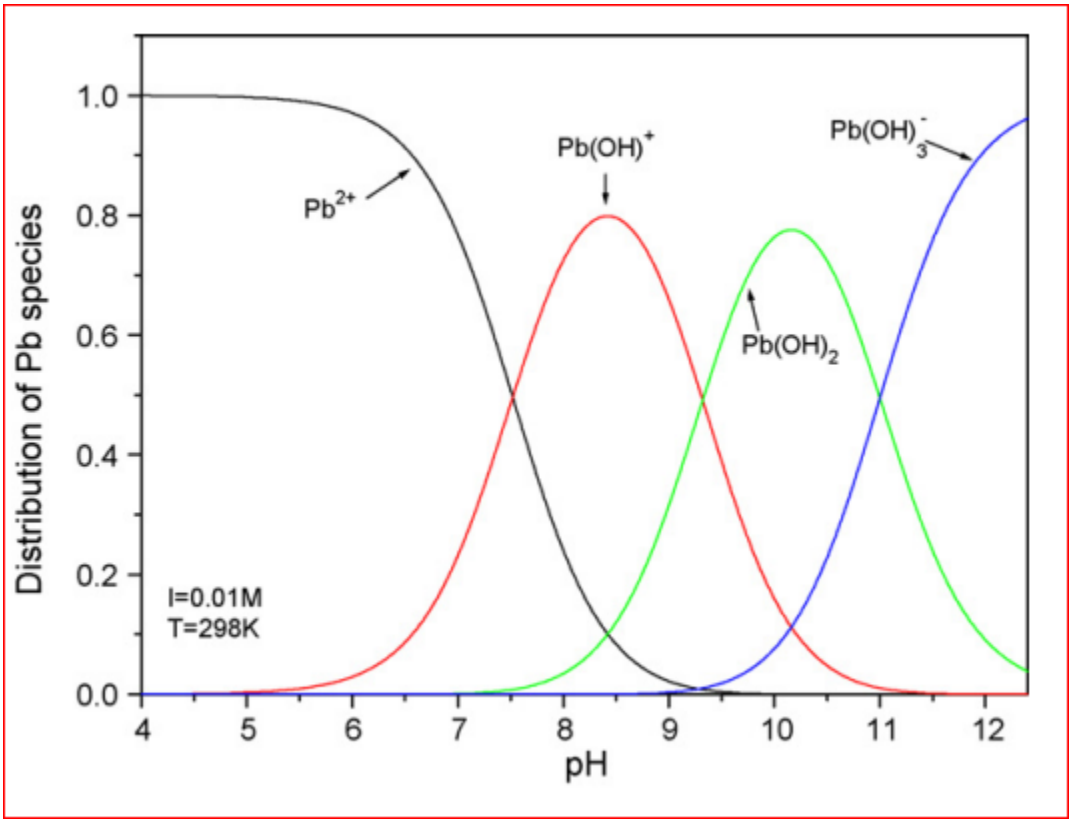

Fig. S1. Distribution of Pb(II) species as a function of pH.

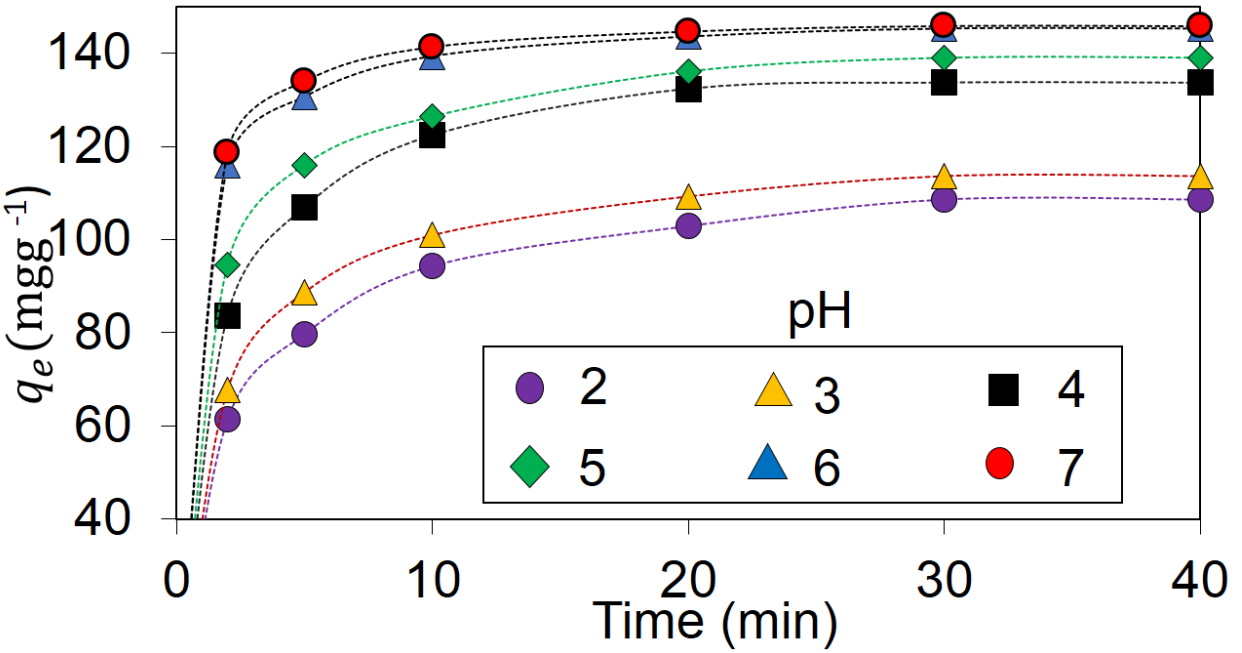

Fig. S2. The effect of pH on the adsorption of Pb(II) ions on $ZnCl_2$-MCM-41 at (C_0=50 mgL^{-1} ; T=20 °C; Sorbent dosage=0.333 gL^{-1}; 300 rpm)

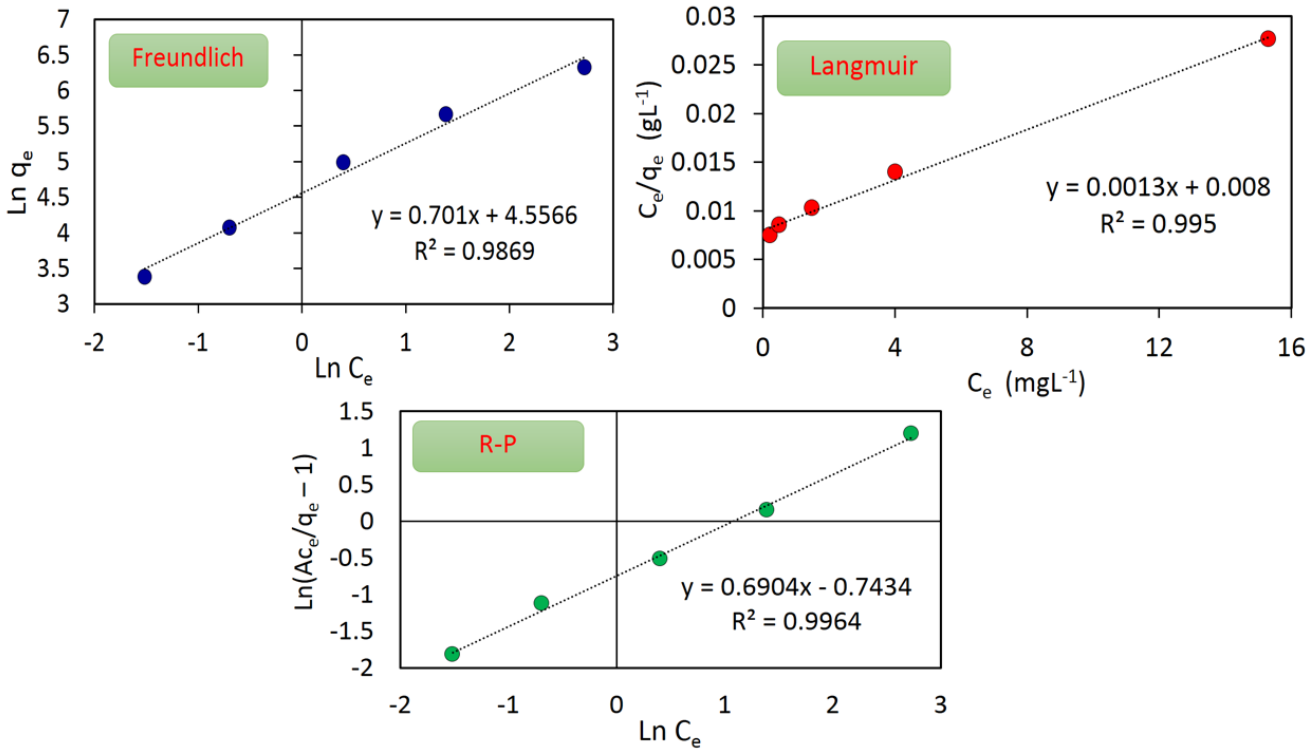

Fig. S3. Adsorption isotherms of Pb(II) removal by $ZnCl_2$-MCM-41