

(Supplementary Section)

Facile synthesis of ZIF-67 incorporated electrospun PVA nanofibers composite for efficient Pb (II) adsorption from water: Docking and experimental studies

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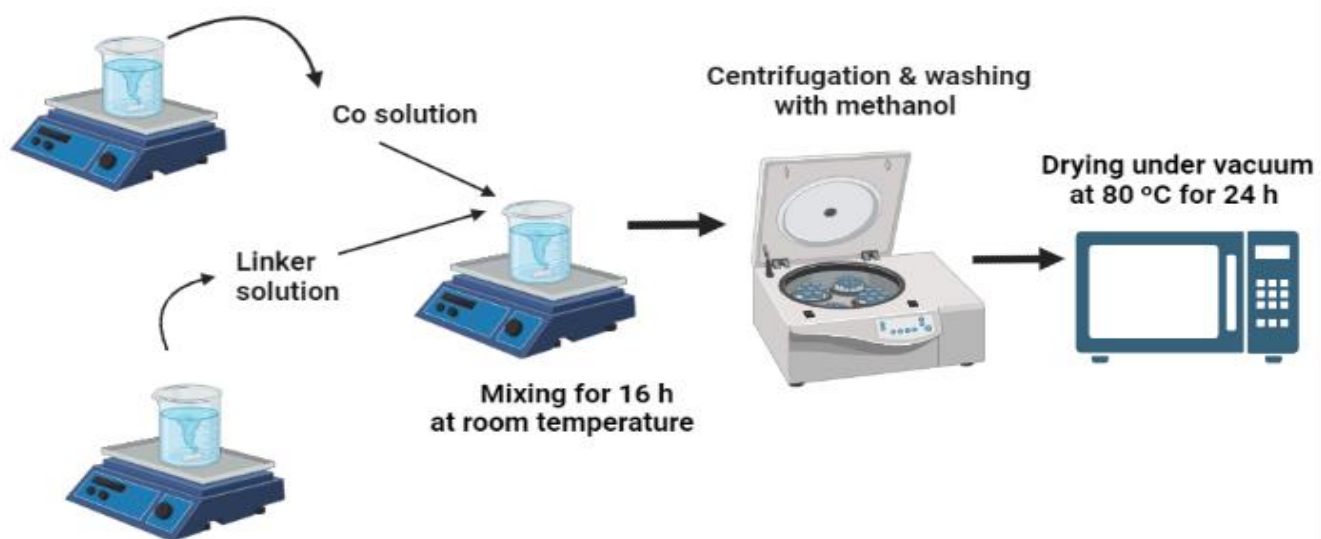
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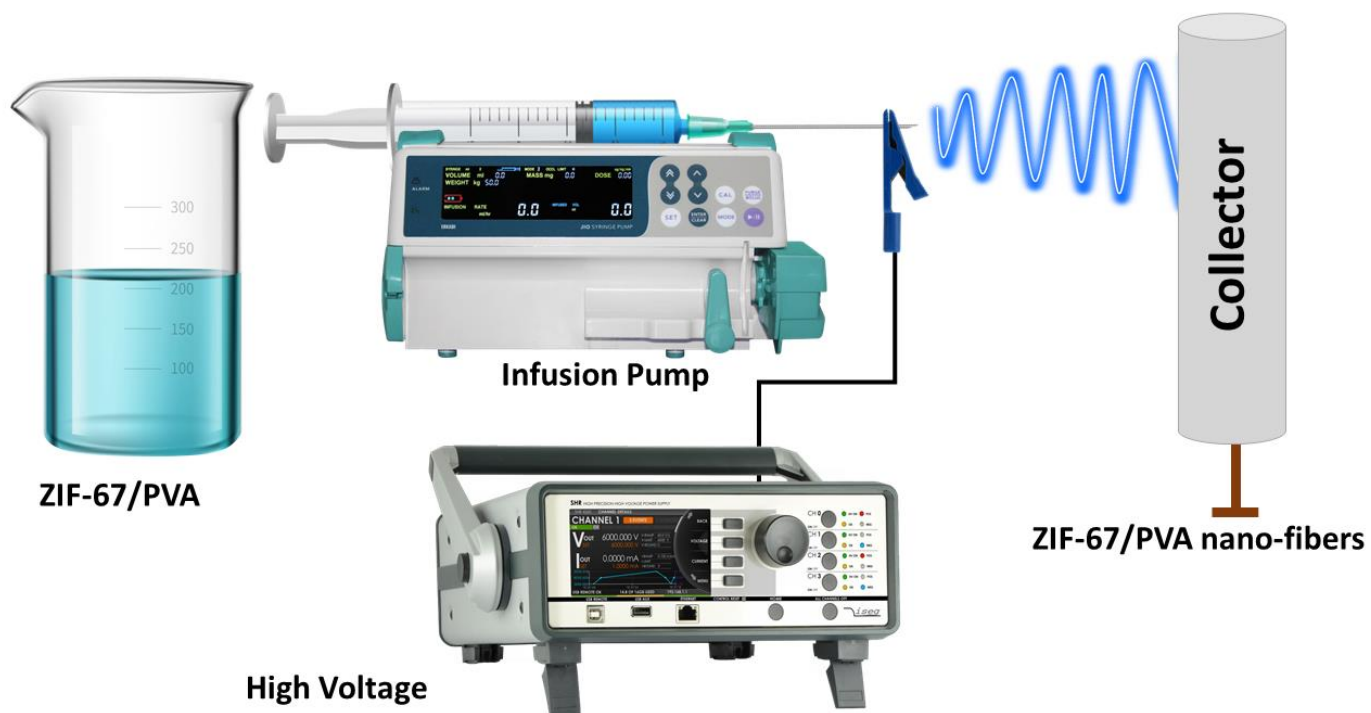
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4 g of $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ in 100 mL methanol



16.8 g of 2- methylimidazole in 100 mL methanol

Scheme S1: A schematic flow diagram for the formation of ZIF-67

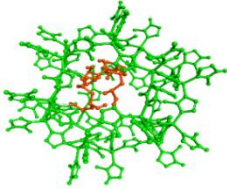
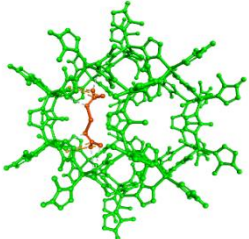
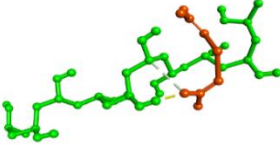
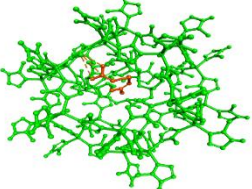


Scheme S2: Synthesis procedure for ZIF-67/PVA nanofibers

Table S1: Systems utilized for molecular docking

System	Macromolecule	Ligand
ZIF67-PVA	ZIF67	PVA
ZIF67-Pb	ZIF67	Pb
PVA-Pb	PVA	Pb
ZIF67-PVA-Pb	ZIF67-PVA	Pb

Table S2. Results obtained using molecular docking simulations for predicting interactions in various systems

System	Topmost Docked Structure*	Binding Energy (Kcal mol ⁻¹)	Type of Interactions
ZIF67-PVA		+1.85	Hydrogen bonding (C-H)
ZIF67-Pb		-2.07	Electrostatic and hydrogen bonding (C-H)
PVA-Pb		-2.90	Hydrogen bonding (conventional and C-H)
ZIF67-PVA-Pb		-3.30	Electrostatic and hydrogen bonding (conventional and C-H)

* Orange: Electrostatic interaction, Light green: C-H Hydrogen bond, Yellow: Conventional Hydrogen bond

Table S3: Calculations of the different kinetic models for Pb (II) sorption onto ZIF-67/PVA nanofibers

Model	C_0	10.0	20.0	30.0	40.0	50.0
Pseudo 1 st order model	K_1	0.030	0.022	0.016	0.004	0.001
	q_e	42.4	63.3	99.4	283.5	1808.7
	R^2	0.98	0.98	0.98	0.97	0.95
Pseudo 2 nd order model	K_2 [g mg ⁻¹ min ⁻¹]	0.0005	0.0002	9.23E-05	0.0001	1.79E-05
	q_e	53.2	84.4	139.6	139.6	303.3
	R^2	0.99	0.99	0.98	0.89	0.89
The Mixed 1, 2-order model	K	0.001	0.0006	0.001	0.0005	4.83E-06
	q_e	52.1	82.8	136.0	446.4	23.39 E4
	f_2	0.961	0.966	0.920	0.805	2.7E-07
	R^2	0.99	0.99	0.99	0.97	0.95
Avrami model	q_e	42.4	63.3	99.4	284.4	6828.8
	k_{av}	0.179	0.154	0.129	0.067	0.013
	n_{av}	0.169	0.145	0.123	0.064	0.013
	R^2	0.98	0.98	0.98	0.97	0.95
Intraparticle diffusion model	k_{ip}	3.88	5.59	7.75	9.20	10.11
	c_{ip}	2.7	0.8	0	0	0
	R^2 [-]	0.98	0.99	0.99	0.91	0.79

Where C_0 in mg/L, K_1 in min⁻¹, q_e in mg g⁻¹, K_2 in g mg⁻¹ min⁻¹, k_{ip} in mg/g.min^{1/2} and c_{ip} in mg g⁻¹

Table S4: Parameters of the isotherm adsorption for the Pb²⁺ sorption to ZIF-67/PVA nanofibers

Model	Parameter	Value	Parameter	Value
Langmuir (linear)	q _{max} [mg. g ⁻¹]	109.9	R ²	0.81
	b	0.37		
Langmuir (non-linear)	q _{max} [mg. g ⁻¹]	364.49	R ²	0.86
	K _L	0.027		
Freundlich (linear)	n	2.297	R ²	0.88
	K _F [Lmg ⁻¹]	30.58		
Freundlich (non-linear)	n	1.56	R ²	0.91
	K _F [Lmg ⁻¹]	18.35		
Dubinin–Radushkevich	q _m [mg. g ⁻¹]	226.73	R ²	0.99
	K _{ad}	0.0024		
Khan	q _m [mg. g ⁻¹]	0.208	a _K	0.361
	b _K	1101	R ²	0.91
Fritz-Schlunder	q _{mFSS} [mg. g ⁻¹]	31.21	m ₁	0.639
	K ₁	0.740	m ₂	0
	K ₂	0.259	R ²	0.91

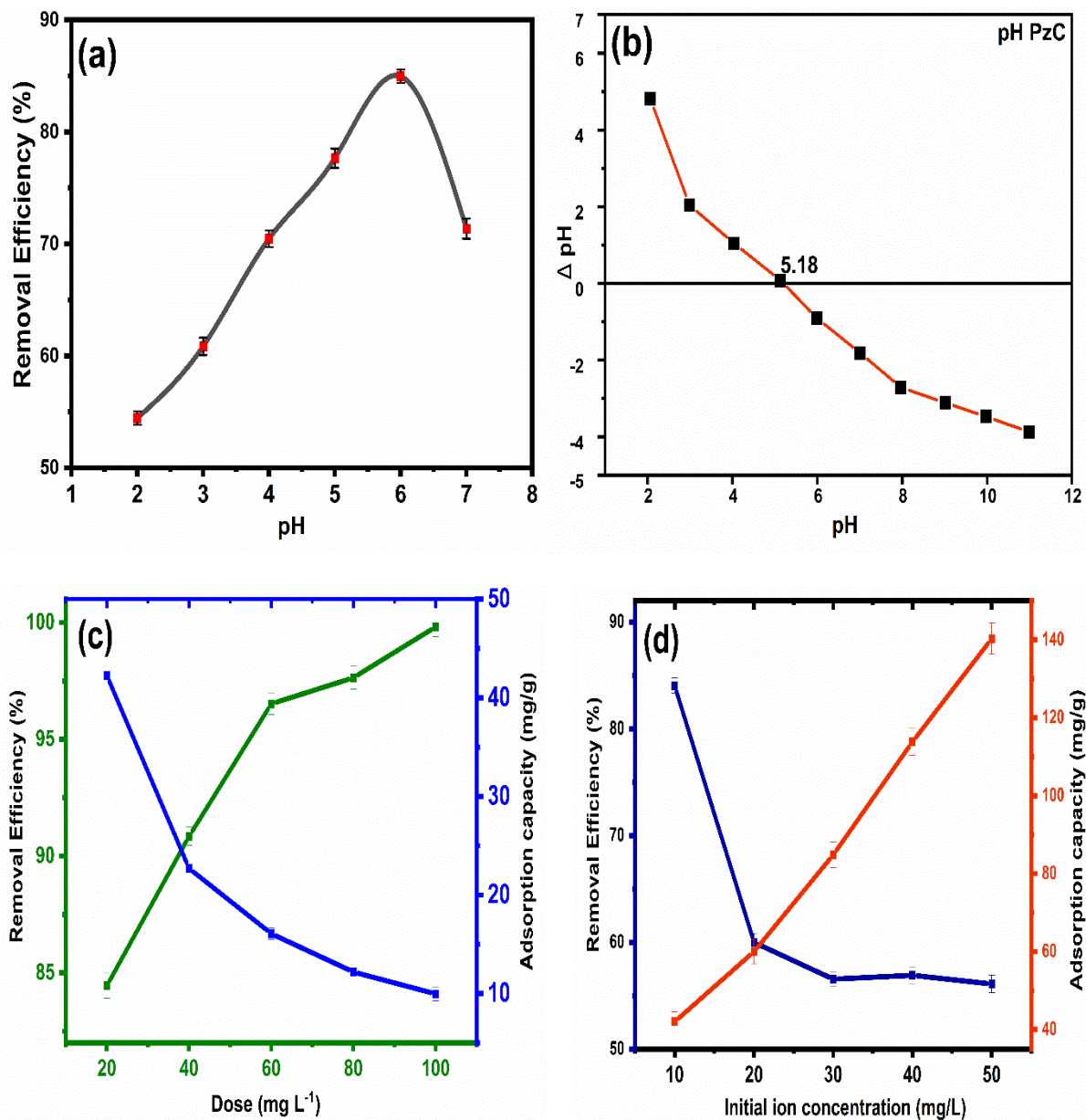


Figure S1. Effect of different parameters on Pb^{2+} adsorption (a) Variation of pH: 2-7 (ZIF-67/PVA nanofibers 20 mg/L, Pb^{2+} concentration 10 mg/L, time of contact 2 h), (b) Point of zero charge (c): Variation of ZIF-67/PVA nanofibers dosage (pH 6, ZIF-67/PVA nanofibers 20-100 mg/L, Pb^{2+} concentration 10 mg/L and time 2 h) & (d) Effect of Pb concentration (pH 6, ZIF-67/PVA nanofibers 20 mg/L, Pb^{2+} concentration 10 - 50 mg/L and time of contact 2 h).

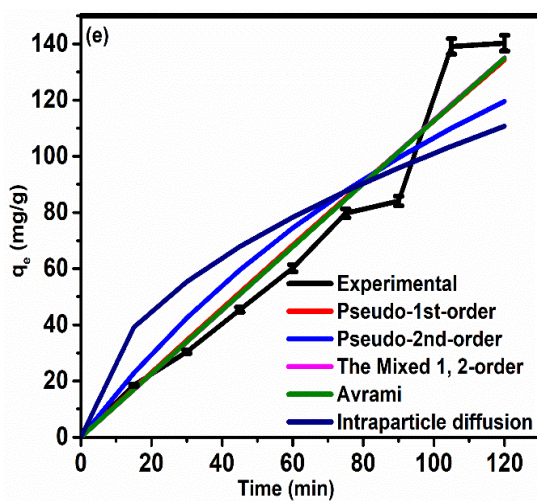
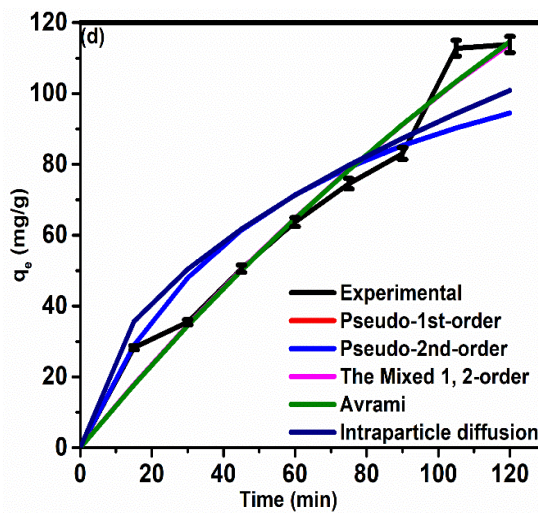
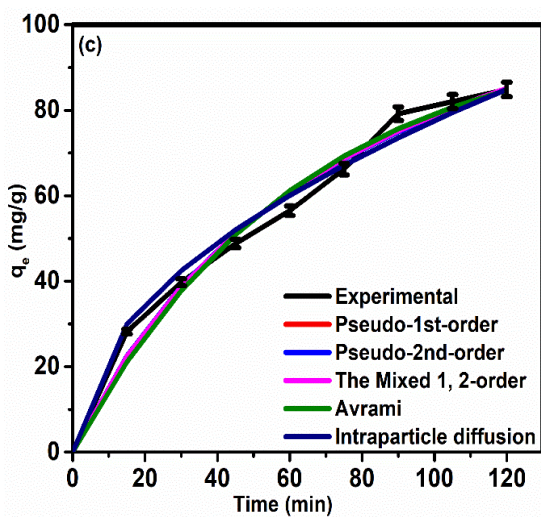
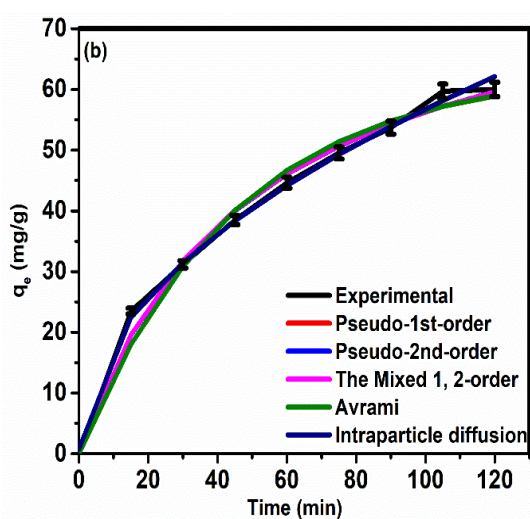
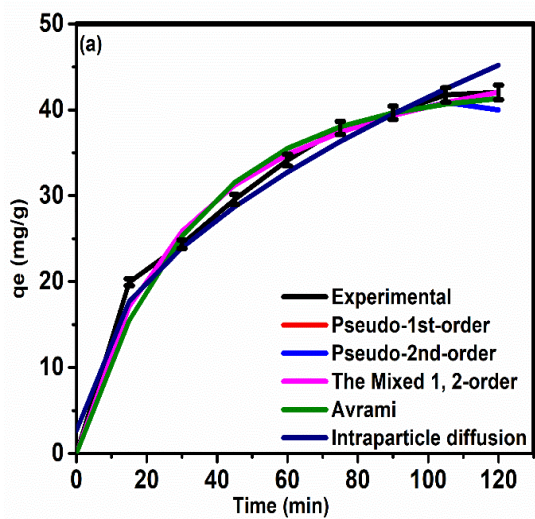


Figure S2. Fitting of the experimental data to the PFO, PSO, IPD, mixed 1st and 2nd order, and Avrami models for Pb²⁺ adsorption onto ZIF-67/PVA nanofibers at different initial concentrations: (a) 10, (b) 20 (c) 30 (d) 40 and (e) 50 mg L⁻¹.

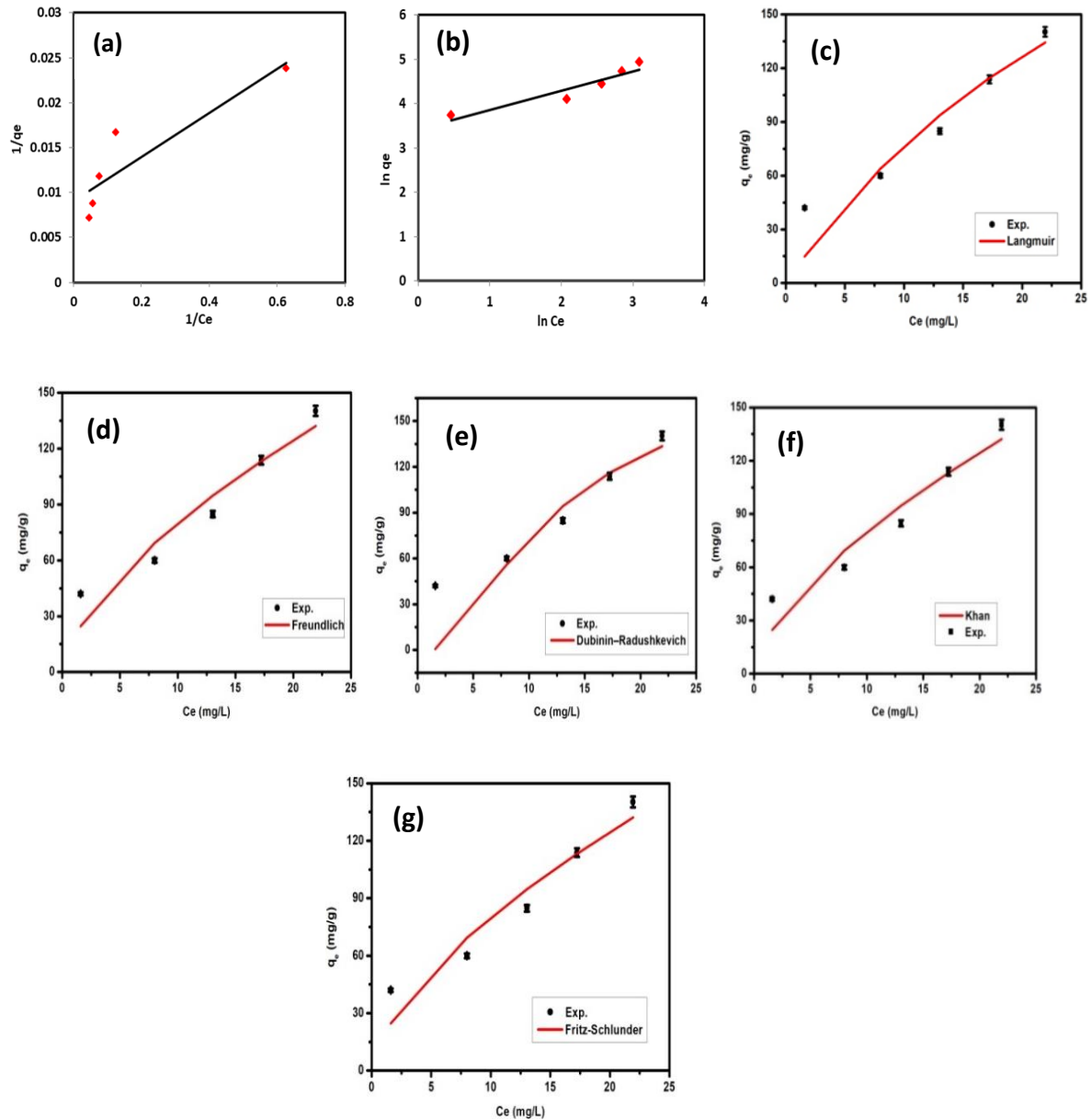


Figure S3. Fitting the experimental data of the Pb²⁺ adsorption onto ZIF-67/PVA nanofibers using: (a) Langmuir (linear), (b) Freundlich (linear), (c) Langmuir (non-linear), (d) Freundlich (non-linear), (e) Dubinin–Radushkevich, (f) Khan, and (g) Fritz-Schlunder models.

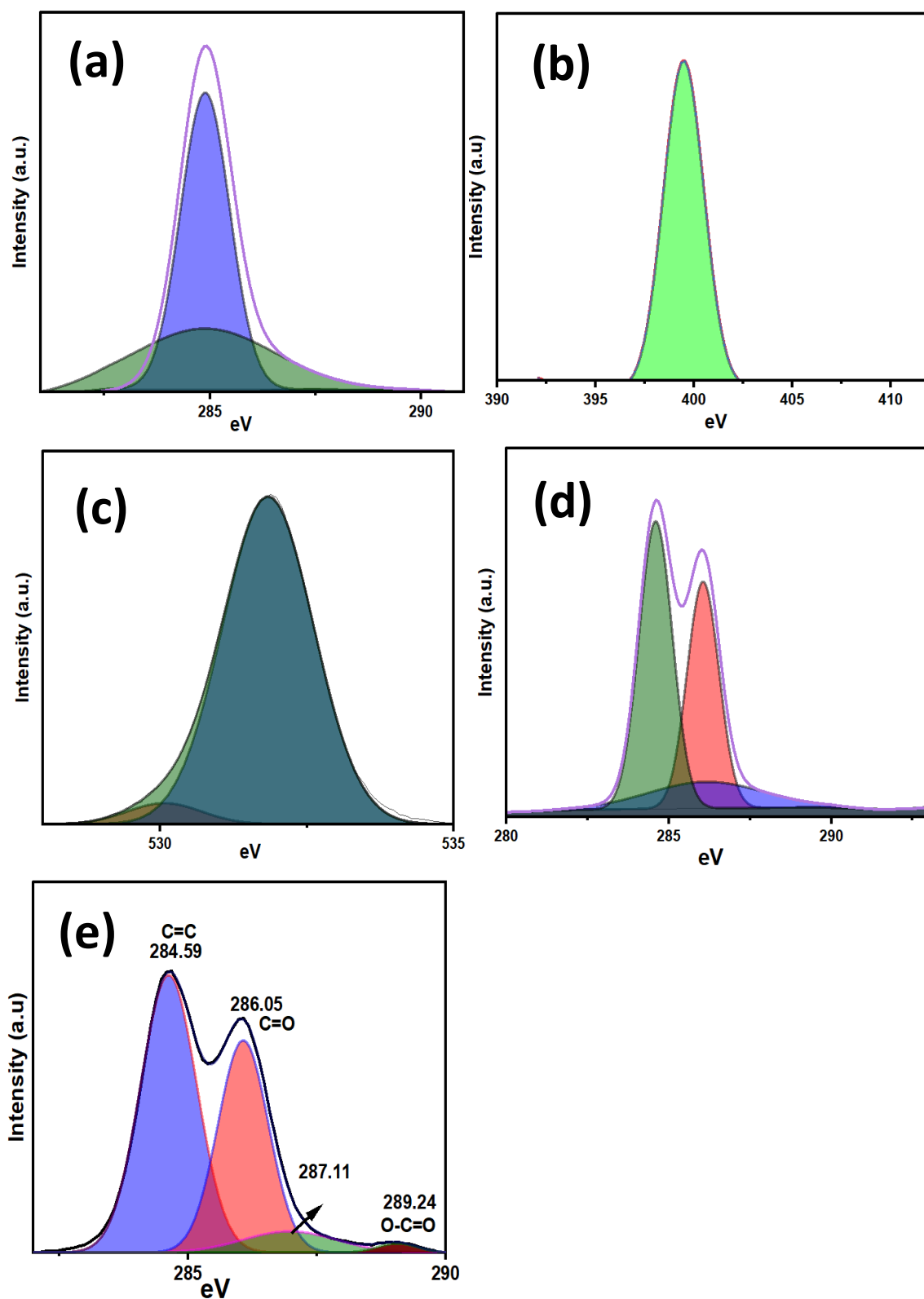


Figure S4. (a) XPS spectra of C 1s in zif-67, (b) N 1s spectrum in zif-67, (c) O 1s spectrum in zif-67, (d): XPs of C after electrospinning and (e) high-resolution spectra of C 1s after Pb (II) adsorption.

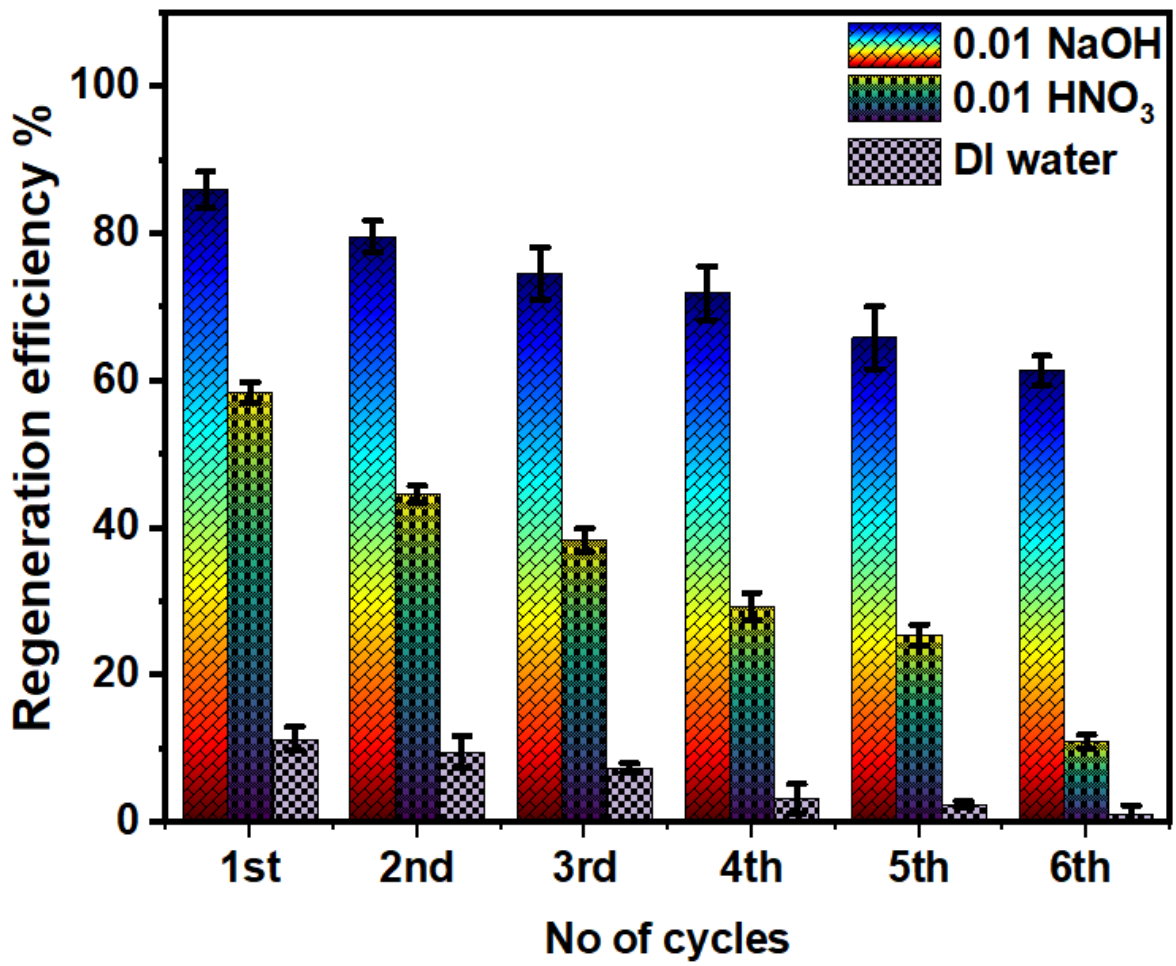


Figure S5: Cyclic stability of ZIF-67/PVA nanofibers after seven cycles