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# Experimental and Theoretical Calculation Investigation on Efficient Pb(II) Adsorption to Etched $Ti_3AlC_2$ Nanofibers and Nanosheets

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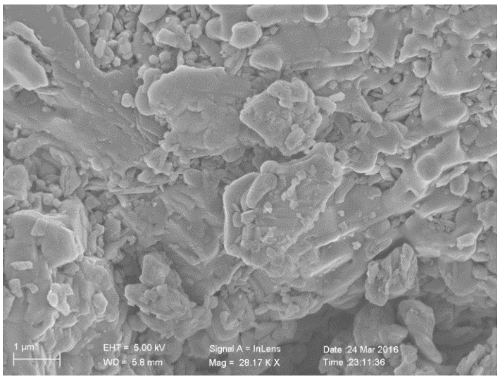


**Fig.** S1. The SEM image of pristine $Ti_3AlC_2$

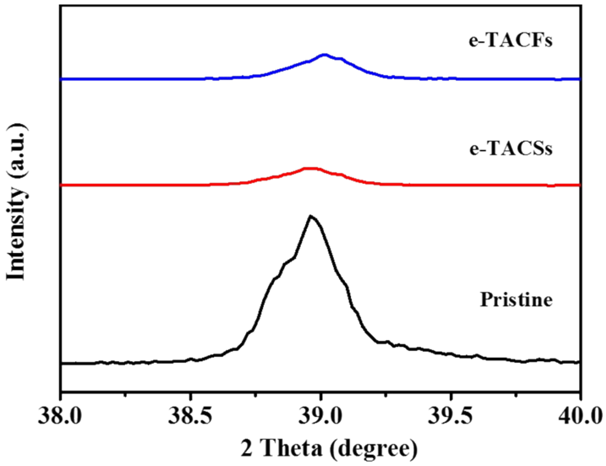


**Fig.** S2. XRD patterns for pristine $Ti_3AlC_2$, e-TACSs and e-TACFs.

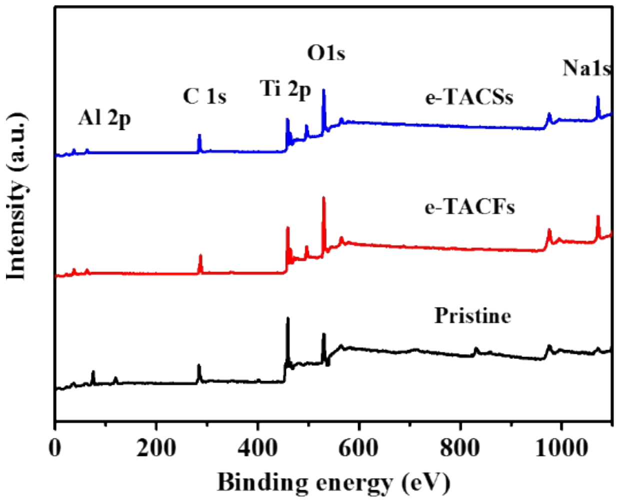


**Fig.** S3. XPS spectra of pristine $Ti_3AlC_2$, e-TACFs and e-TACSs.

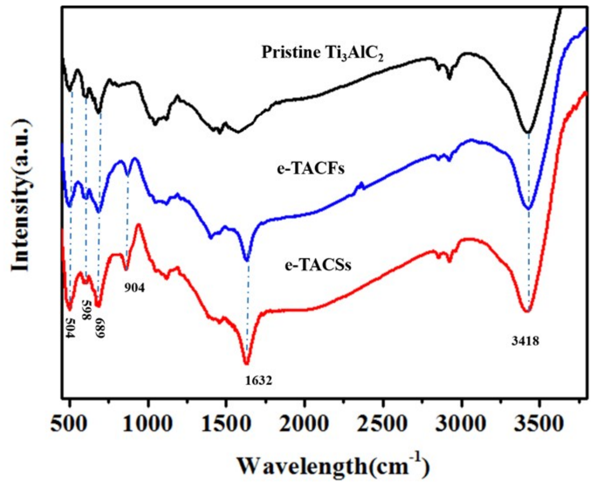


**Fig.** S4. FT-IR spectra of pristine $Ti_3AlC_{2,}$ e-TACFs and e-TACSs.

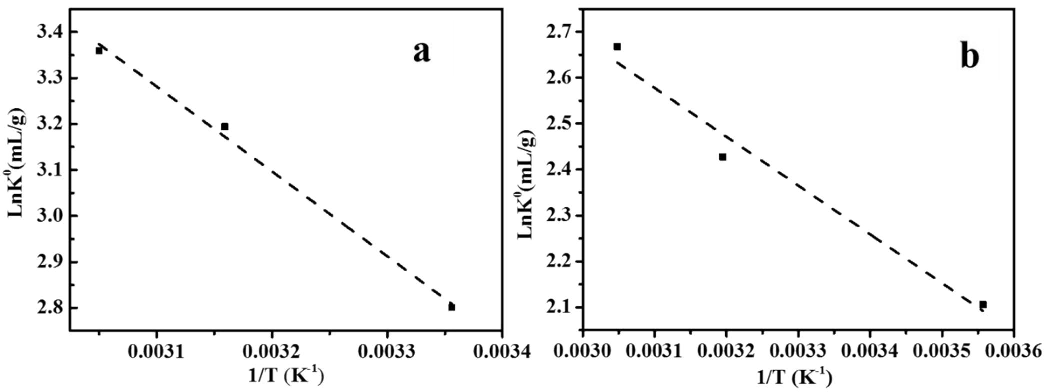


**Fig.** S5 Linear plot of 1/T to $\ln K_0$ for the adsorption of Pb(II) onto e-TACFs (a) and e-TACSs (b).

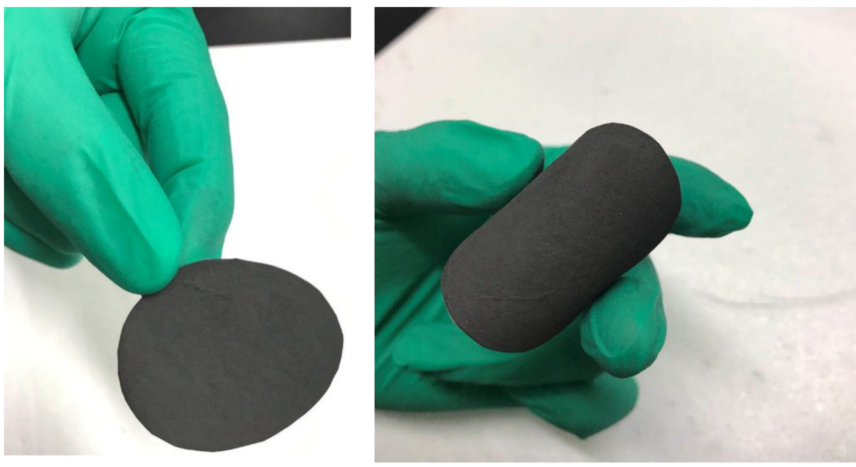

Fig. S6 The construction of free-standing e-TACFs membrane.

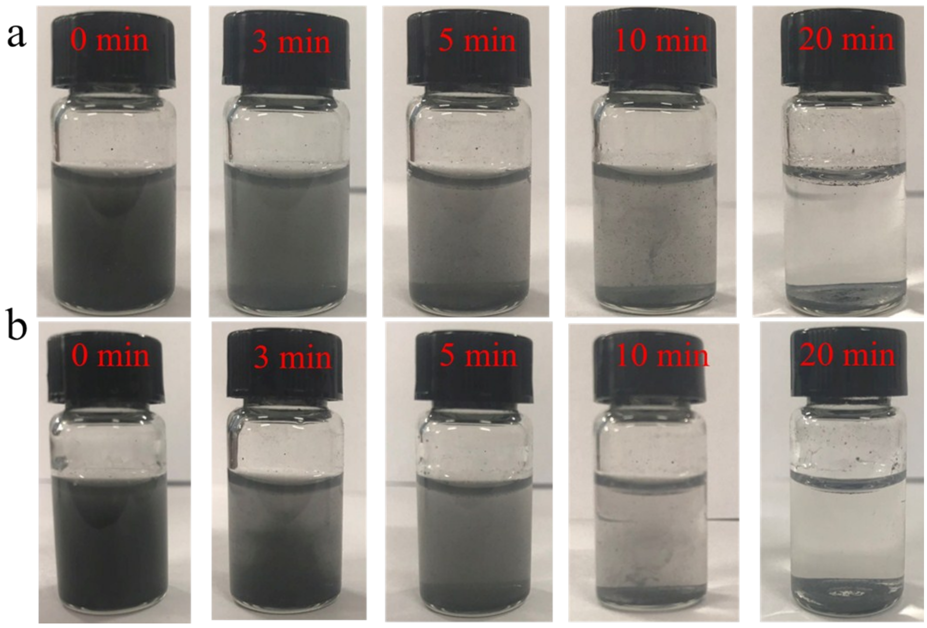


Fig. S7 Static settling properties in various time intervals of e-TACFs (a), e-TACFs (b) with the process of lead uptake.

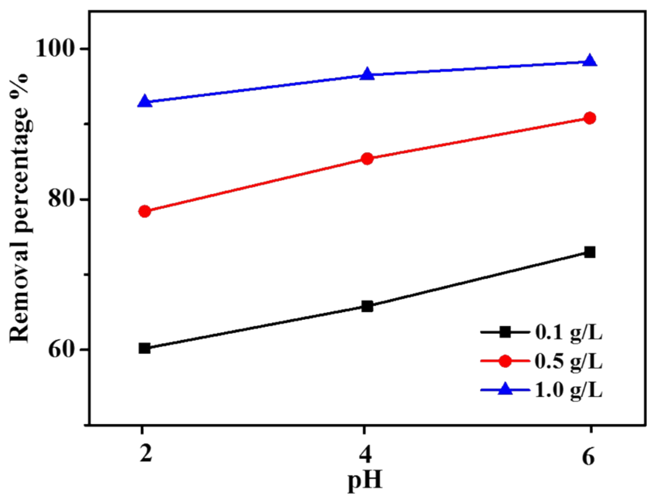


Fig. S8 Effect of pH and solid content on Pb(II) sorption to e-TACFs. Conditions: $C(Pb)_{initial}$ = 20 mg $L^{-1}$, m/V = 0.1, 0.5 and 1.0 mg $L^{-1}$, I = 0.001 M and T = 298 K.

**Table** S1. The detailed surface elements of pristine $Ti_3AlC_2$ e-TACSs and e-TACFs.

| Element | element % | | | | |
|---|---|---|---|---|---|
| | Ti | Al | C | O | Na |
| $Ti_3AlC_2$ | 47.2 | 18.7 | 22.4 | 10.7 | - |
| e-TACFs | 22.7 | 2.8 | 18.7 | 46.5 | 9.60 |
| e-TACSs | 25.7 | 2.6 | 24.2 | 30.27 | 7.27 |

**Notes:** - No corresponding element signals detected.

**Table** S2. Comparison of the thermodynamic parameters and adsorption capacities of Pb(II) with previous related studies at 298 K.

| Adsorbents | Experimental condition | | | Sorption capacity (mg/g) | Ref. |
|---|---|---|---|---|---|
| | pH | T (K) | m/V (g/L) | | |
| Na-bentonite | 4.0 | 298 | 0.5 | 47.8 | 1 |
| Sporopollenin | 6.0 | 298 | - | 8.5 | 2 |
| Iron oxide | 5.5 | 298 | 10 | 36.0 | 3 |
| $g$-$C_3N_4$/β-CD | 5.5 | 298 | 0.3 | 100.1 | 4 |
| e-TACSs | 5.0 | 298 | 0.2 | 218.3 | This study |
| e-TACFs | 5.0 | 298 | 0.2 | 285.9 | This study |

**Table** S3. Parameters for the kinetic adsorption data simulated by pseudo-first-order and pseudo-second-order models

| Adsorbents | Pseudo-first-order | | | Pseudo-second-order | | |
|---|---|---|---|---|---|---|
| | $q_e$ mg/g | $k_1$ min$^{-1}$ | $R^2$ | $q_e$ mg/g | $k_2$ min$^{-1}$ | $R^2$ |
| e-TACFs | 162.7 | 0.09531 | 0.905 | 166.3 | 0.00583 | 0.938 |
| e-TACSs | 147.4 | 0.04805 | 0.764 | 153.4 | 0.00113 | 0.941 |

**Table** S4. The detailed surface elements of e-TACFs and e-TACSs before and after Pb(II) removal

| Samples | element % | | | | | |
|---|---|---|---|---|---|---|
| | Ti | Al | C | O | Na | Pb |
| e-TACFs | 22.7 | 2.89 | 18.7 | 46.7 | 9.60 | - |
| e-TACFs-Pb | 19.96 | 2.52 | 29.66 | 46.01 | 0.21 | 1.44 |
| e-TACSs | 25.7 | 2.61 | 24.15 | 30.27 | 7.27 | - |
| e-TACFs-Pb | 27.37 | 2.49 | 34.47 | 32.46 | 0.27 | 0.7 |

**Table** S5. Binding energies of elements in e-TACFs and e-TACSs before and after Pb(II) adsorption.

| Peaks $E_B$ (eV) | O 1s | | Ti 2p | Na 1s | Pb 4f | |
|---|---|---|---|---|---|---|
| | Ti-O | Ti-OH (%) | | | Pb $4f_{5/2}$ | Pb $4f_{7/2}$ |
| e-TACFs | 530.0 | 532.0 (22.1%) | 458.4 eV | 1072.1eV | - | - |
| e-TACFs-Pb | 530.6 | 532.6(12.8%) | 459.0 eV | - | 143.9 eV | 139.1 eV |
| e-TACSs | 530.0 | 532.0 (16.2%) | 458.4 eV | 1072.1eV | - | - |
| e-TACFs-Pb | 530.3 | 532.3 (14.6%) | 458.7 eV | - | 143.9 eV | 139.1 eV |

# Reference

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