

Supplementary Information

Electrospun Nanofibers of 2D Cr_2CT_x MXene Embedded in PVA for Efficient Electrocatalytic Water Splitting

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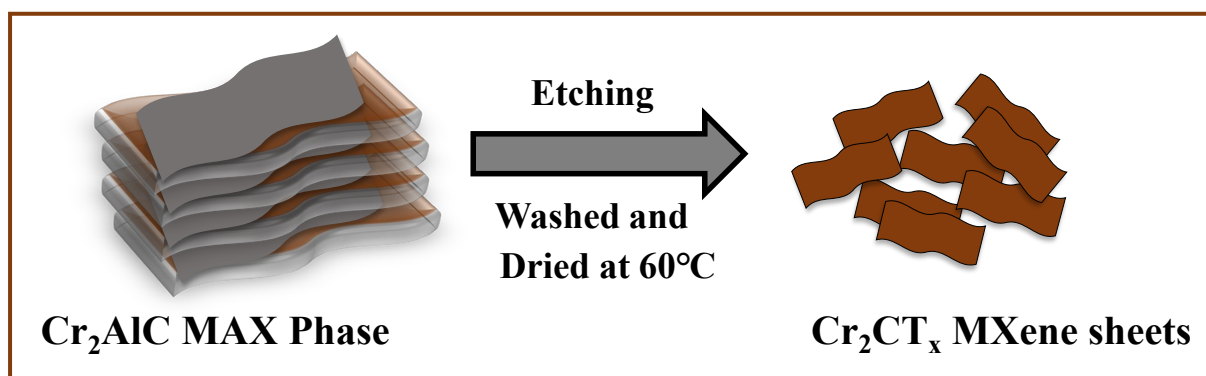


Fig. S1. Schematic illustration of the synthesis of Cr_2CT_x MXene sheets

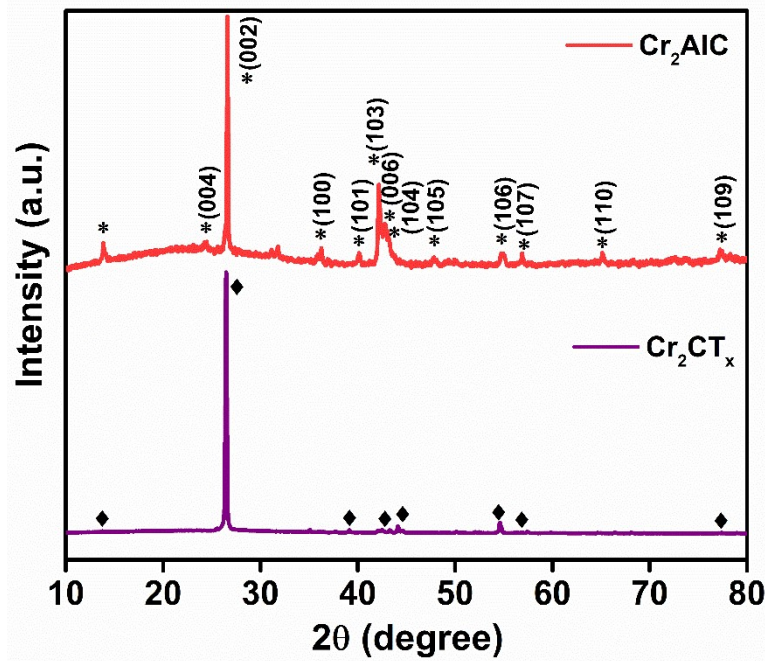


Fig. S2. XRD of Cr_2AlC MAX Phase and Cr_2CT_x MXene

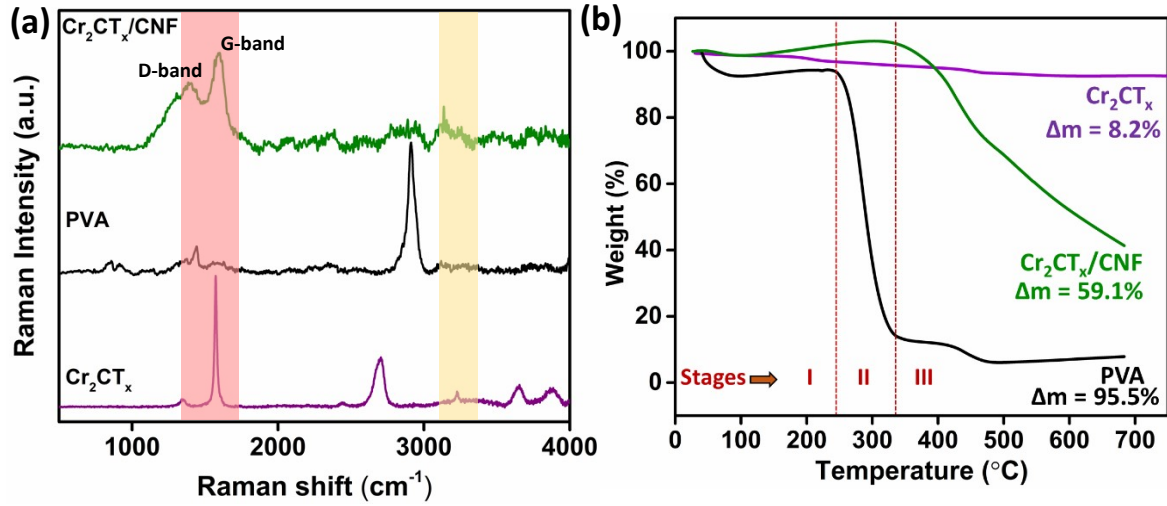


Fig. S3. (a) Raman spectra and (b) TGA profiles of $\text{Cr}_2\text{CT}_x/\text{CNF}$, PVA, and Cr_2CT_x

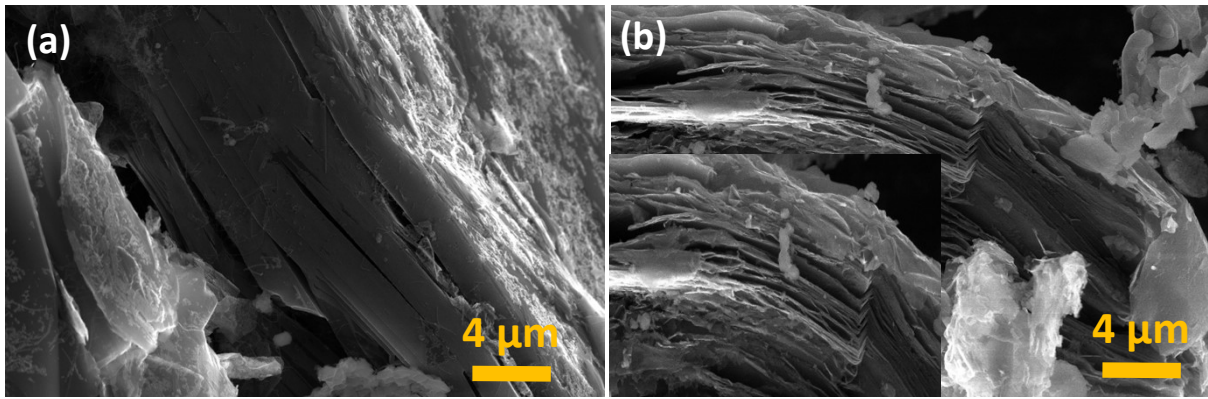


Fig. S4. SEM image of (a) Cr₂AlC MAX Phase (b) Cr₂CT_x MXene

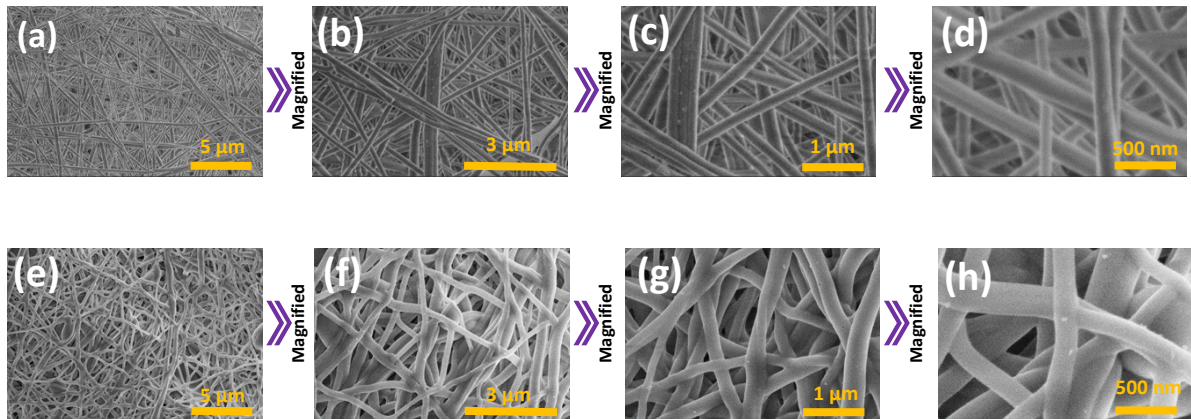


Fig. S5. SEM images of (a-d) Cr₂CT_x/CNF1 and (e-h) Cr₂CT_x/CNF

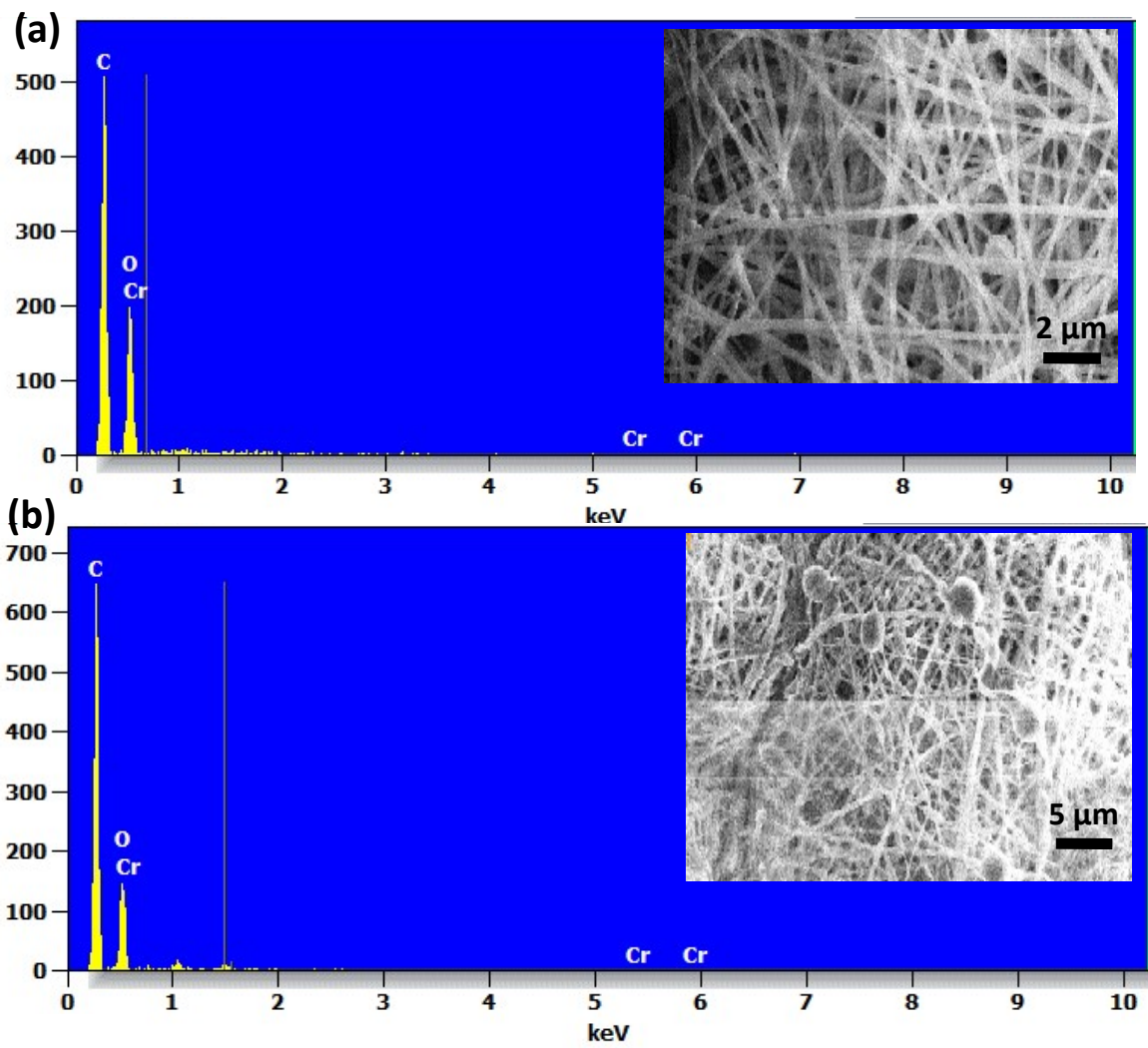


Fig. S6. EDX spectra (inset SEM image) of (a) $\text{Cr}_2\text{CT}_x/\text{CNF1}$ and (b) $\text{Cr}_2\text{CT}_x/\text{CNF}$

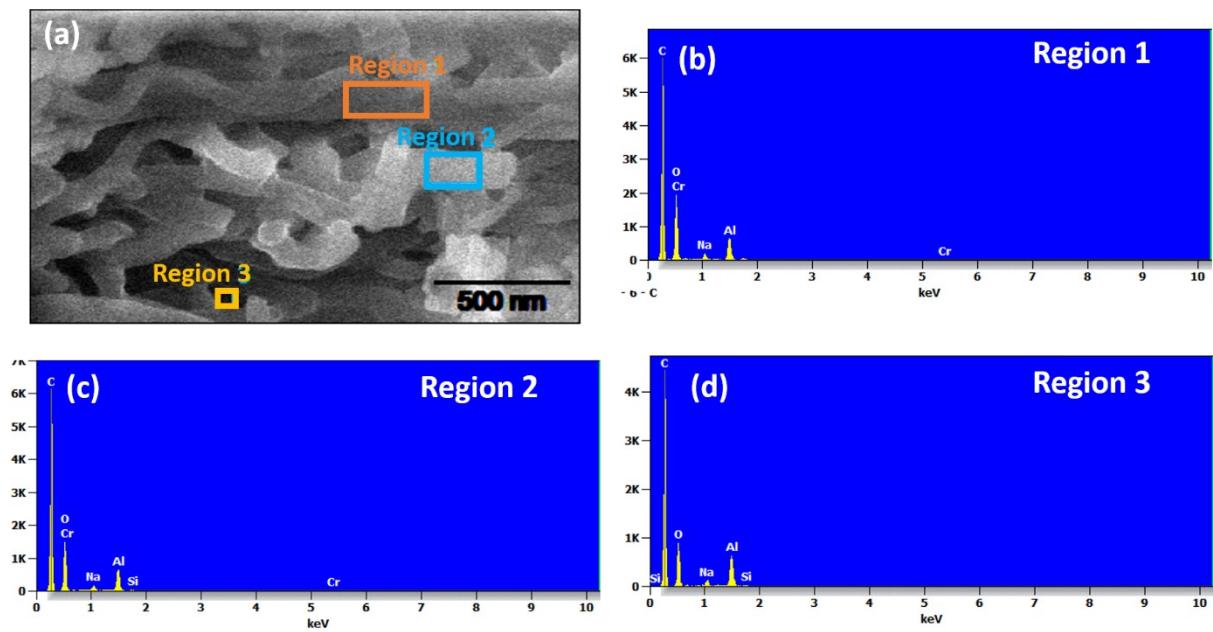


Fig. S7. Cross-sectional SEM images of $\text{Cr}_2\text{CT}_x/\text{CNF}$ with various regions within the fiber matrix (regions 1 and 2) and outside the fiber matrix (region 3), Area EDX spectrum of $\text{Cr}_2\text{CT}_x/\text{CNF}$ analyzed in (a) region 1, (b) region 2 and (c) region 3.

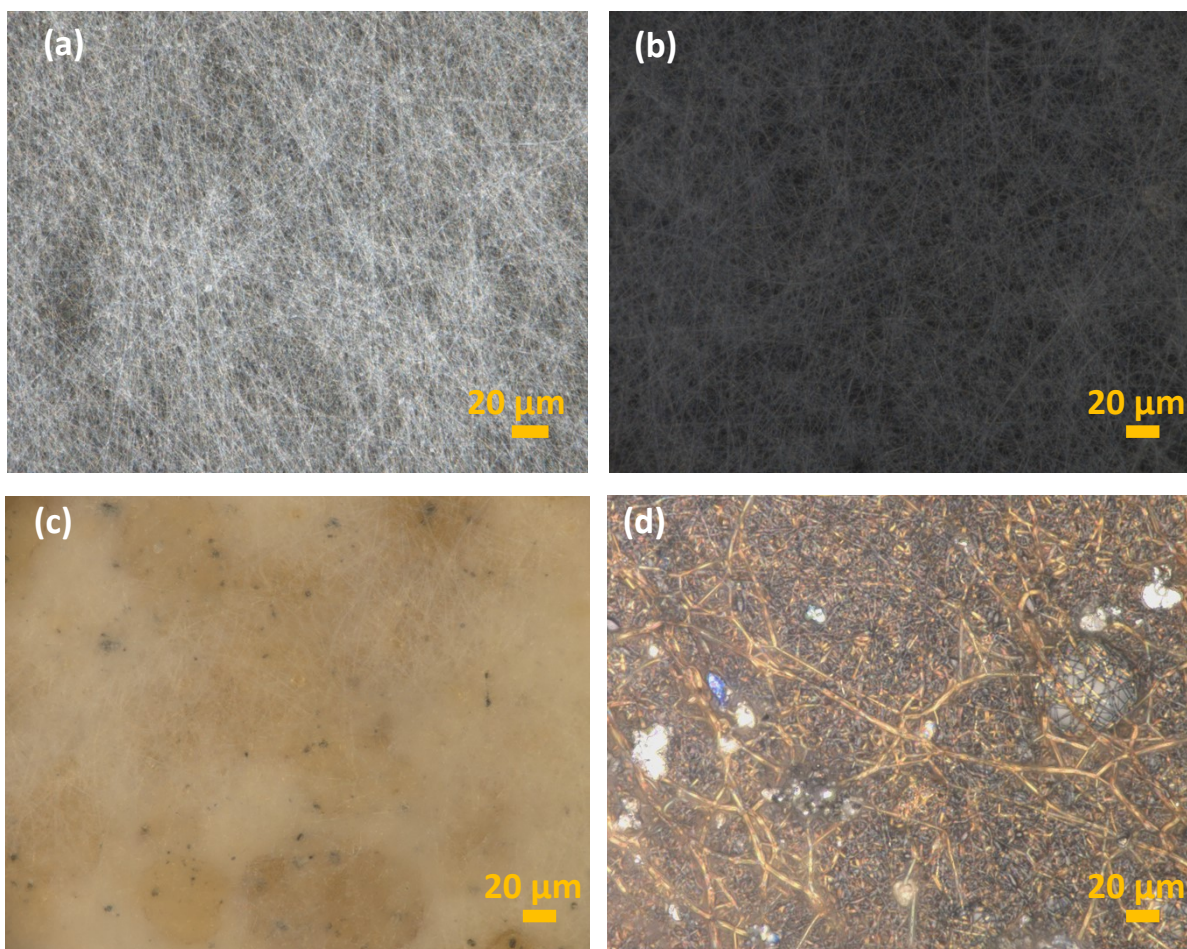


Fig. S8. Optical microscopic images of nanofiber mats of (a) PVA, (b) Cr_2CT_x /PVA, (c) Cr_2CT_x /CNF1 and (d) Cr_2CT_x /CNF

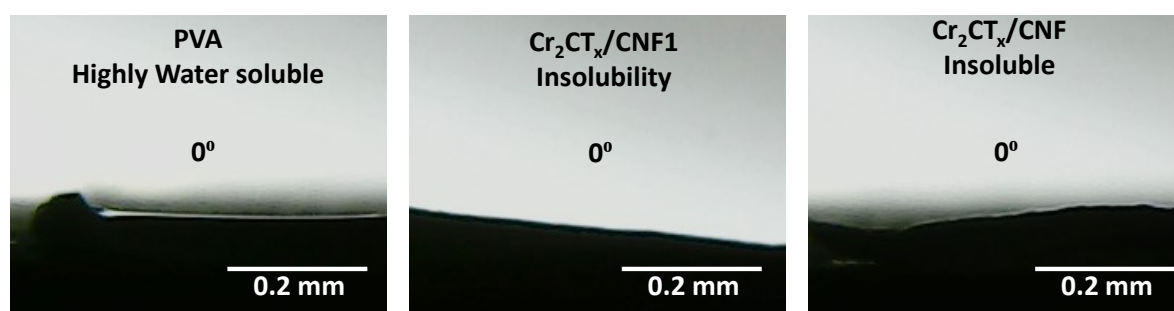


Fig. S9. Surface wettability of nanofiber samples. Magnified photographs of water droplets placed over the fibrous mats are shown in the images.

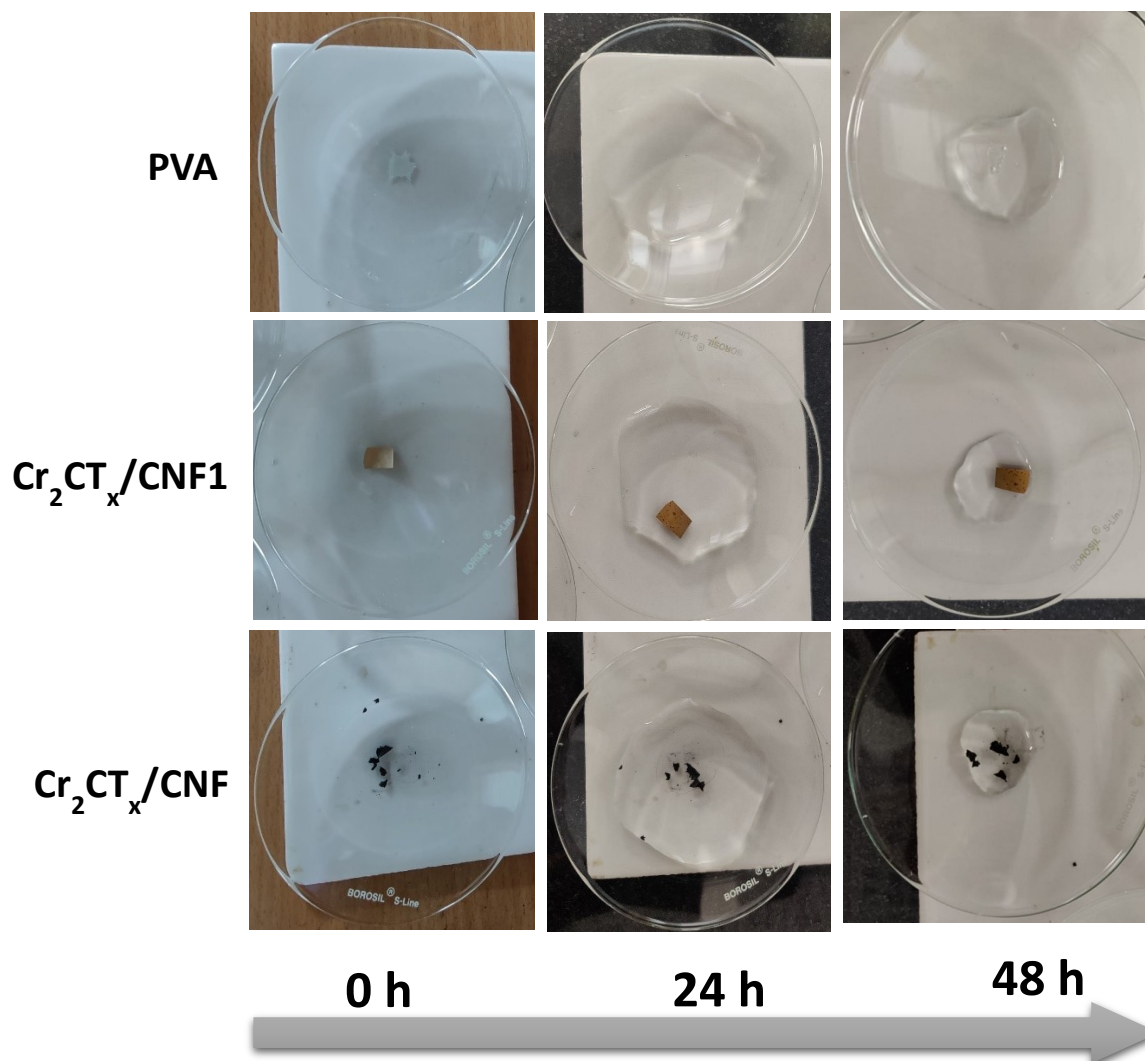


Fig. S10. Photographs showing the water Solubility of PVA, $\text{Cr}_2\text{CT}_x/\text{CNF1}$ and $\text{Cr}_2\text{CT}_x/\text{CNF}$ with time.

Video S1. Evidence for the insolubility of $\text{Cr}_2\text{CT}_x/\text{CNF}$ compared the PVA nanofibrous mat.

(Uploaded separately)

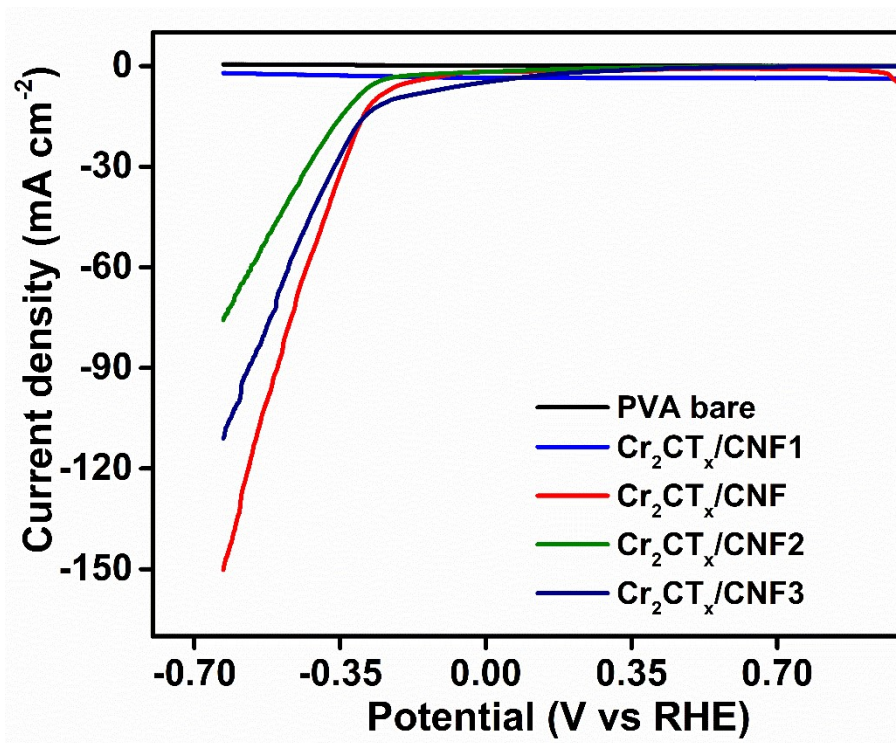


Fig. S11. Comparison of LSV profiles of PVA bare and various $\text{Cr}_2\text{CT}_x/\text{CNF}$ obtained for HER

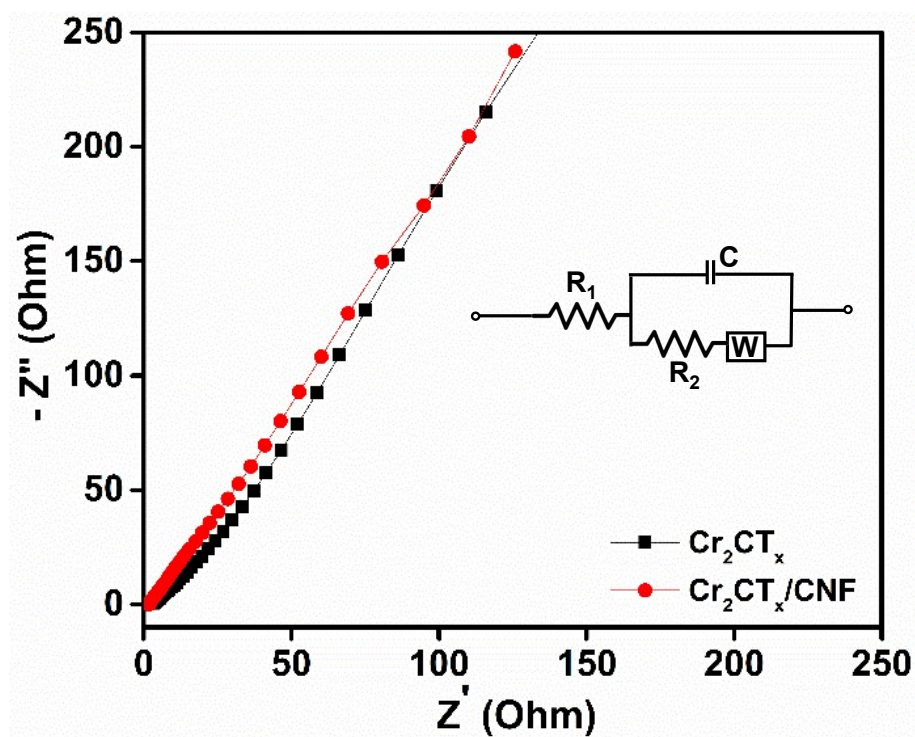


Fig. S12. Nyquist plot with fitted Randles circuit for HER performance

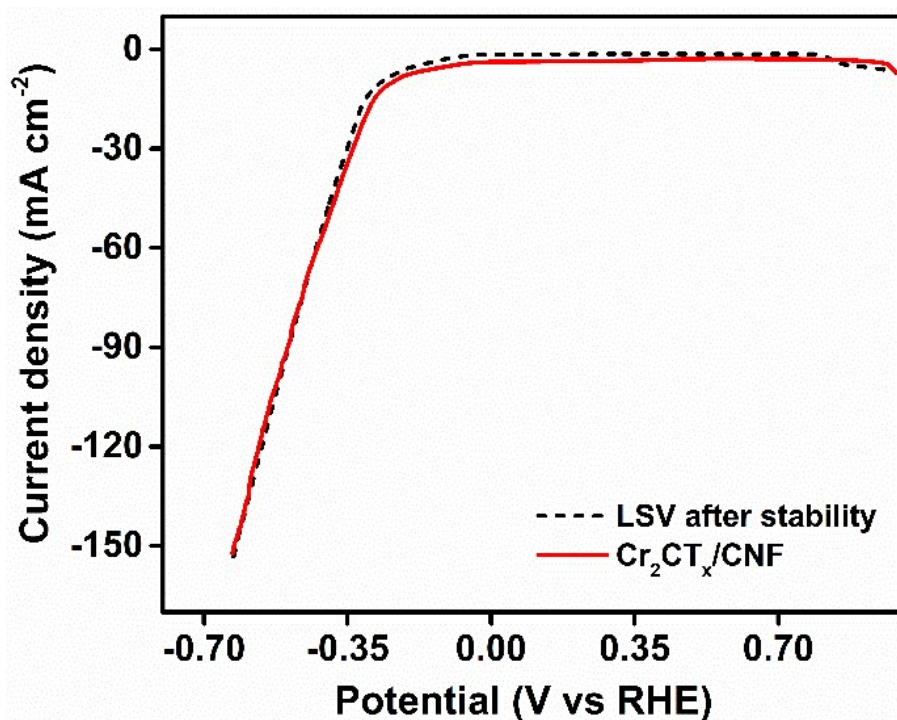


Fig. S13. LSV profile of $\text{Cr}_2\text{CT}_x/\text{CNF}$ before and after stability check for HER

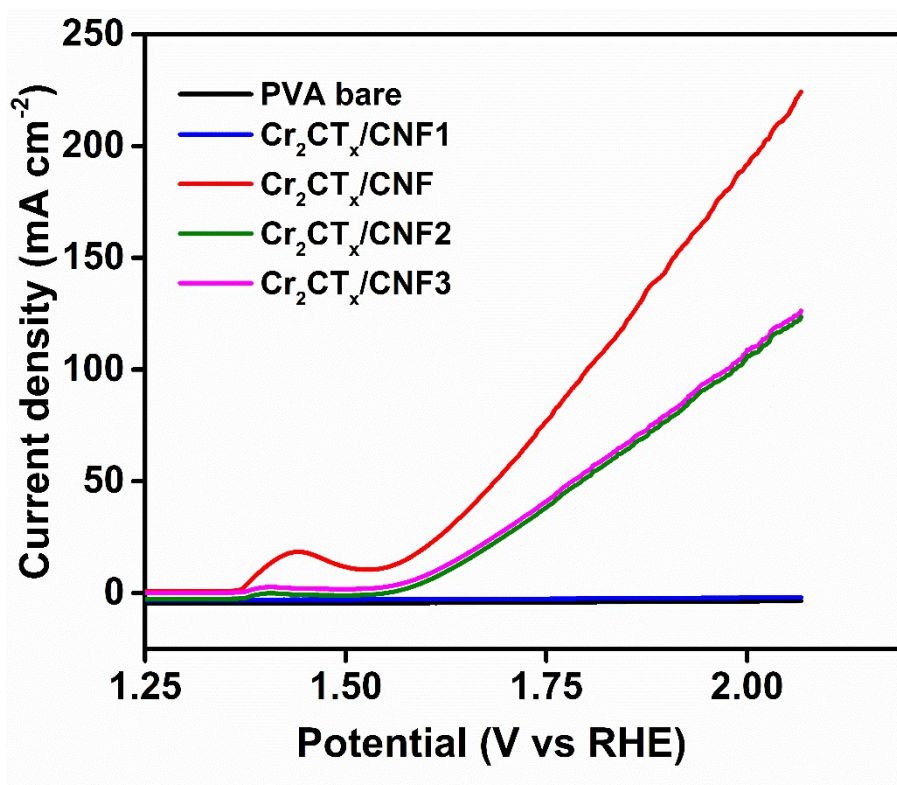


Fig. S14. Comparison of LSV profiles of PVA bare and various $\text{Cr}_2\text{CT}_x/\text{CNF}$ obtained for HER

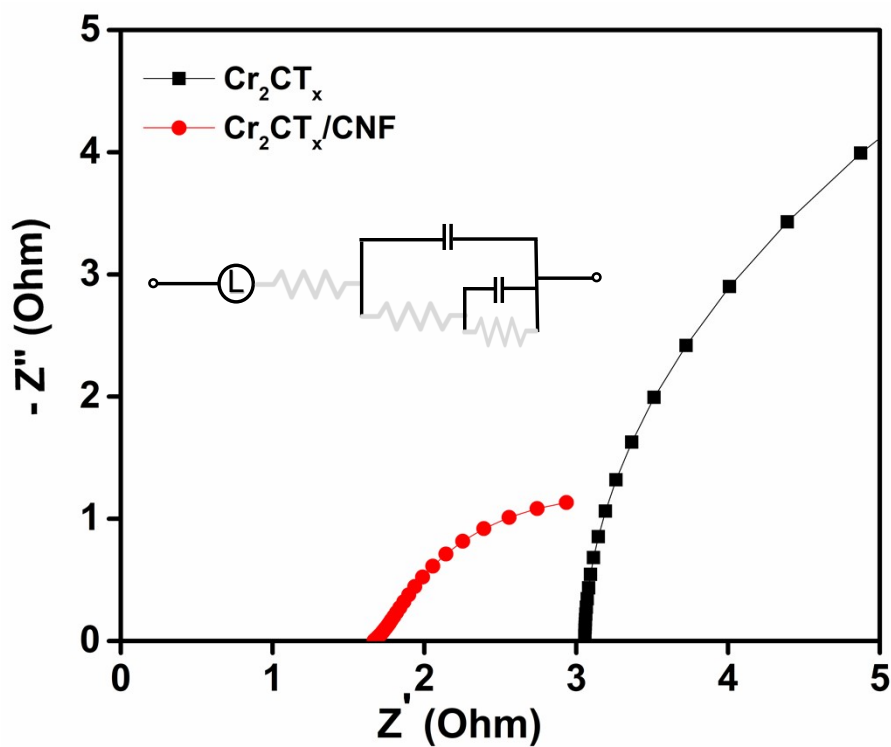


Fig. S15. Nyquist plot fitted Randles circuit for OER performance

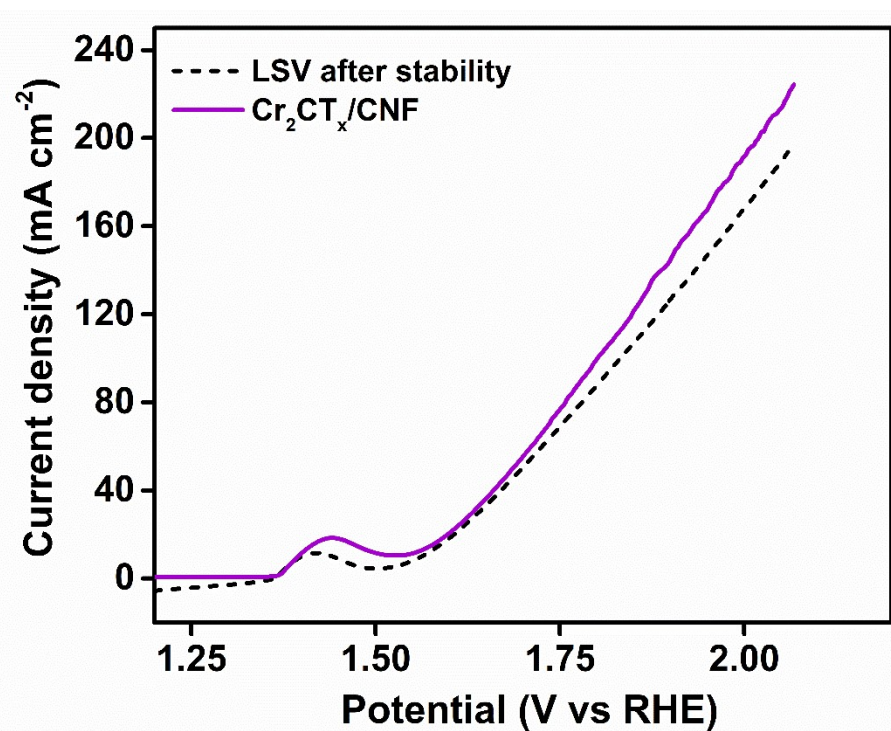


Fig. S16. LSV profile of Cr₂CT_x/CNF before and after stability check for OER

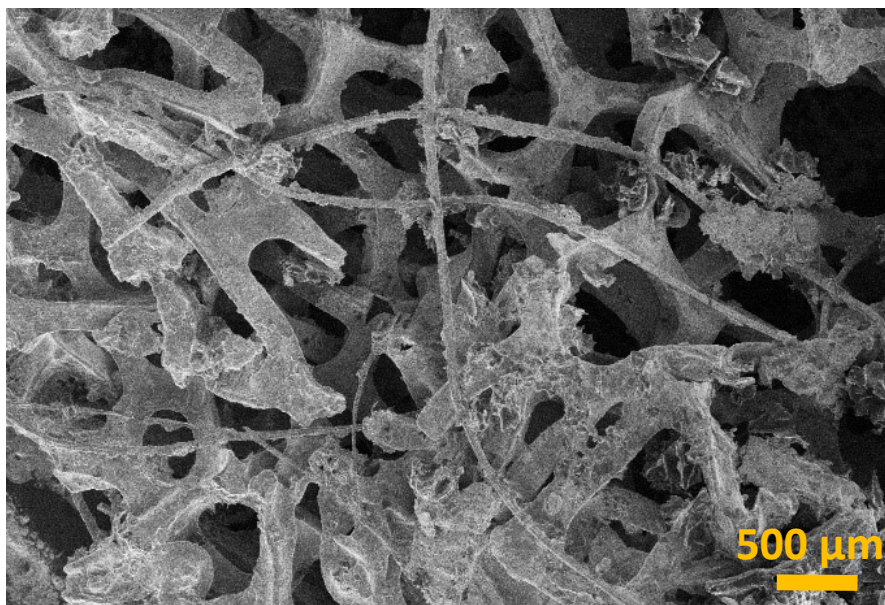


Fig. S17. SEM image of $\text{Cr}_2\text{CT}_x/\text{CNF}$ after bulk electrolysis (stability test)

Table S1. Elemental compositions derived from the EDX analysis of prepared $\text{Cr}_2\text{CT}_x/\text{CNF1}$ and $\text{Cr}_2\text{CT}_x/\text{CNF}$

| Materials | Element present | Weight % | Atom % | Atom % Error |
|--------------------------------------|-----------------|----------|--------|--------------|
| $\text{Cr}_2\text{CT}_x/\text{CNF1}$ | C | 43.21 | 51.91 | ±0.74 |
| | O | 51.79 | 46.71 | ±1.04 |
| | Cr | 4.99 | 1.39 | ±0.33 |
| $\text{Cr}_2\text{CT}_x/\text{CNF}$ | C | 50.03 | 57.20 | ±0.71 |
| | O | 49.83 | 42.76 | ±1.05 |
| | Cr | 0.14 | 0.04 | ±0.07 |

Table S2. The weight and atomic percentage of elements present in the Cr₂CT_x/CNF were analyzed in various regions as shown in Fig. S7

| Position | Parameter | C | O | Cr | Al | Na | Si |
|------------------------------------|--------------|-------|-------|-------|-------|-------|-------|
| Region 1 (within fiber matrix) | Weight % | 56.62 | 25.98 | 7.32 | 8.71 | 1.36 | - |
| | Atom % | 68.71 | 23.67 | 2.05 | 4.71 | 0.86 | - |
| | Atom % Error | ±0.49 | ±2.51 | ±0.22 | ±0.12 | ±0.11 | - |
| Region 2 (within fiber matrix) | Weight % | 57.34 | 26.97 | 3.73 | 9.48 | 2.20 | 0.28 |
| | Atom % | 68.31 | 24.12 | 1.03 | 5.03 | 1.37 | 0.14 |
| | Atom % Error | ±0.41 | ±1.73 | ±0.11 | ±0.07 | ±0.08 | ±0.03 |
| Region 3 (outside fiber matrix) | Weight % | 53.20 | 33.41 | - | 11.50 | 1.89 | - |
| | Atom % | 63.04 | 29.72 | - | 6.06 | 1.17 | - |
| | Atom % Error | ±0.41 | ±0.47 | - | ±0.10 | ±0.08 | - |

Table S3. Comparison of HER, OER and OWS activity with reported literature.

| Electrocatalyst | Polymer and Synthesis approach | Reference electrode | Water splitting activity @10 mV cm ⁻² | Ref. |
|---|----------------------------------|---------------------|--|---------------------|
| Sn/Mo ₂ C/CNF | PAN/DMF solution Electrospinning | Hg/HgO | 144 mV -HER | 1 |
| Co ₃ W ₃ C/CoP/N, P-Carbon fibers | PAN/DMF Electrospinning | - | 139 mV -HER 200 mV - OER | 2 |
| S,N-CNF/Co-NiO | PAN/DMF Electrospinning | Hg/HgO | 169 mV - HER 247 mV - OER | 3 |
| NiCo/CNF/N-doped carbon shell | Polydopamine Electrospinning | Hg/HgO | 220 mV - HER 0.40 V - OER | 4 |
| Cr₂CT_x/CNF | PVA Electrospinning | SCE | 265 mV - HER 250 mV - OER | Present work |

References

- 1 L. Zhang, K. Wei, J. Ma, J. Wang, Z. Liu, R. Xing and T. Jiao, *Appl. Surf. Sci.*, 2021, **566**, 150754.
- 2 Y. Zhang, W. Shi, L. Bo, Y. Shen, X. Ji, L. Xia, X. Guan, Y. Wang and J. Tong, *Chem. Eng. J.*, 2022, **431**, 134188.
- 3 S. Surendran, S. C. Jesudass, G. Janani, J. Y. Kim, Y. Lim, J. Park, M. Han, I. S. Cho and U. Sim, *Adv. Mater. Technol.*, DOI:10.1002/admt.202200572.
- 4 T. T. Gebremariam, F. Chen, Y. Jin, Q. Wang, J. Wang and J. Wang, *Catal. Sci. Technol.*, 2019, **9**, 2532–2542.