

Supplementary Information

Molten salt shielded solid-state synthesis (MS⁵) reaction driven >99 % pure Ti₃AlC₂ MAX phase: Effect of MAX phase purity on interlayer separation of MXene and Na-ion storage

Ekta Choudhary,^{a,b} Vishesh Manjunath,^a Ramchandra Kalubarme,^c Ravindra Jangir,^{d,e*} and Rupesh S. Devan,^{a,f,g*}

^aDepartment of Metallurgical Engineering and Materials Science, Indian Institute of Technology Indore, Simrol, Khandwa Road, Indore, 453552, India

^bDepartment of Physics, Indian Institute of Technology Indore, Simrol, Khandwa Road, Indore, 453552, India

^cCentre for Materials for Electronics Technology, Pune, 411008, India

^dAccelerator Physics and Synchrotrons Utilization Division, Raja Ramanna Centre for Advanced Technology, Indore 452013, India

^eHomi Bhabha National Institute, Anushakti Nagar, Mumbai, 400094, India

^fCentre for Electric Vehicle & Intelligent Transport System, Indian Institute of Technology Indore, Simrol, Khandwa Road, Indore, 453552, India

^gMultidisciplinary Academic Research Centre, National Dong Hwa University, Hualien 974301, Taiwan.

*Corresponding authors: email: rjangir.cat@gmail.com & rupesh@iiti.ac.in

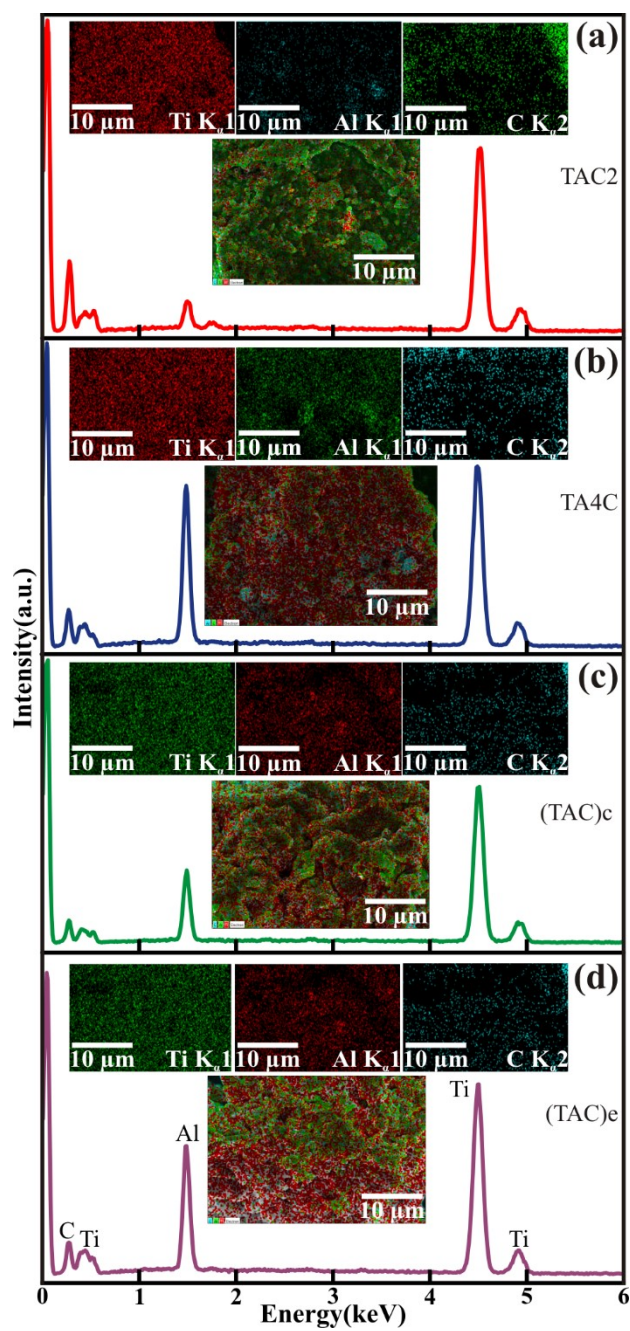


Figure S1. EDS spectra and the corresponding elemental mapping of (a) TAC2, (b) TA4C, (c) (TAC)6, and (d) (TAC)c showing the difference in elemental concentration of $TiK_{\alpha 1}$, $AlK_{\alpha 1}$, and $CK_{\alpha 2}$ with varying the precursor weight ratio, holding time and temperature.

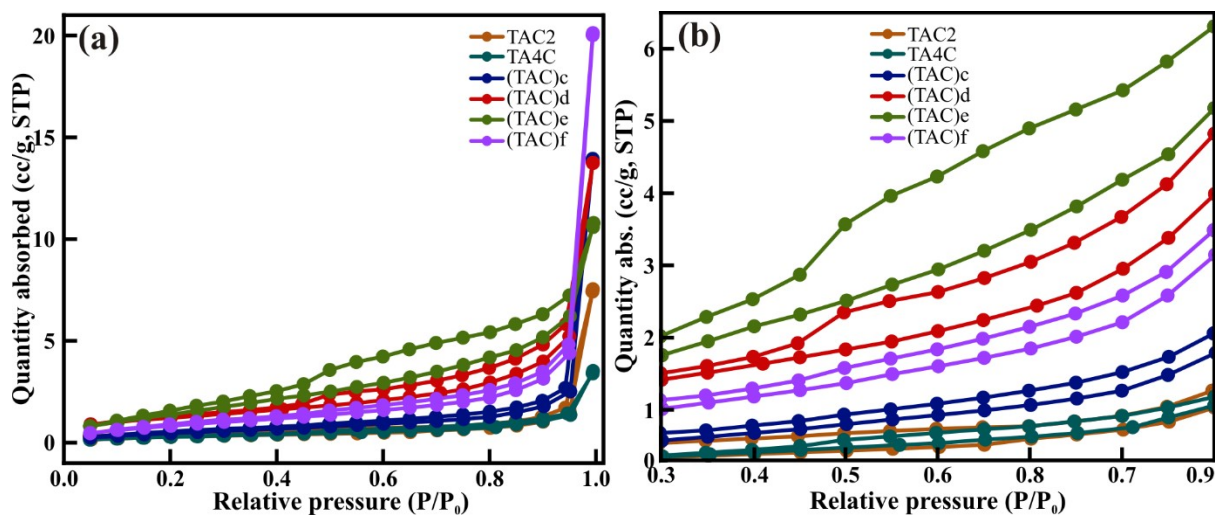


Figure S2. (a) BET curves and (b) their magnified image in the relative pressure 0.3-0.9 P/P₀ of various MAX phases prepared by varying weight ratio, reaction temperature, and time of the molten salt solid-state reaction from which BET surface area is evaluated.

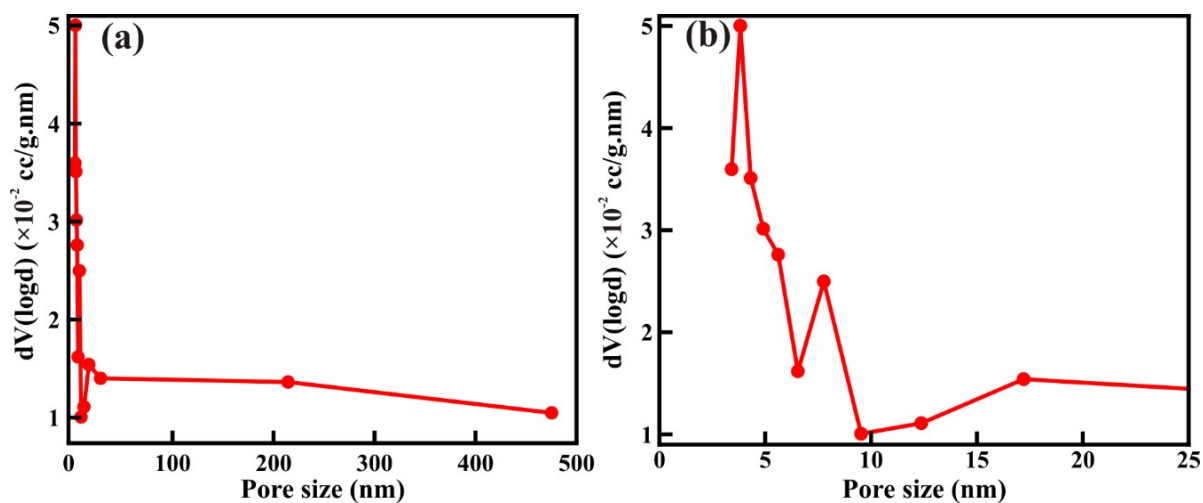


Figure S3. (a) BJH pore size distribution and (b) magnified view till 20 nm for 2D Ti₃C₂-F MXenes obtained from HF etching of optimized (TAC)e MAX phase.

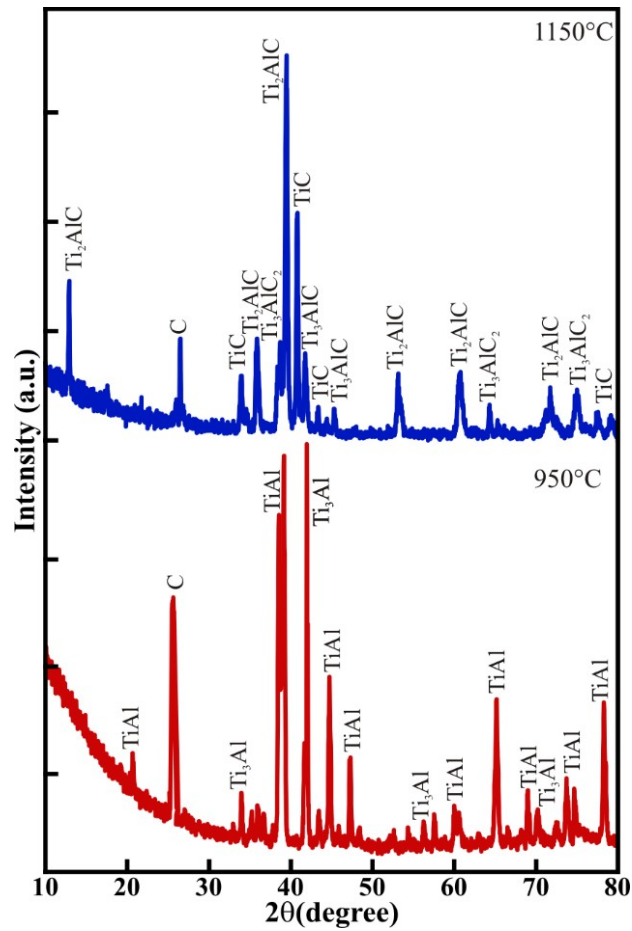


Figure S4. XRD pattern at 950 °C and 1150 °C temperature.

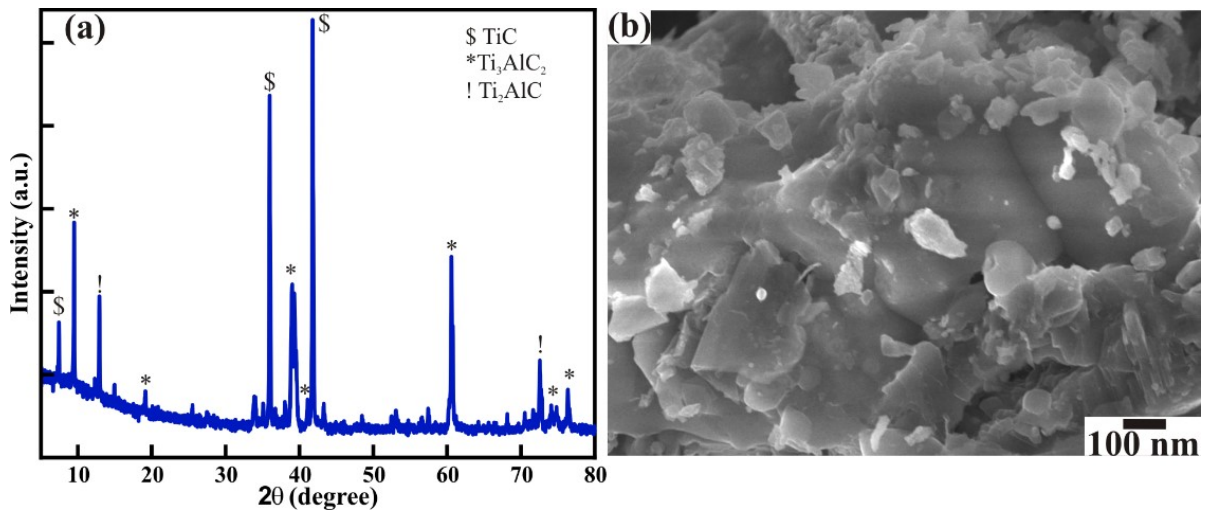


Figure S5. (a) XRD pattern, and (b) FESEM image of Ti_3AlC_2 MAX phase processed at 1400 °C temperature.

Table S1. Comparison of Ti₃C₂-F MXene Performance in Na-ion Batteries

Material	Capacity	Rate	Cyclic stability	Ref.
Ti ₃ C ₂ -T _x	100 mAh g ⁻¹	30 mA g ⁻¹	Retention after 50 cycles	[1]
Ti ₃ C ₂ -T _x	79 mAh g ⁻¹	0.2 A g ⁻¹	Retention after 500 cycles	[2]
Ti ₃ C ₂ -T _x	68.3 mAh g ⁻¹	0.2 A g ⁻¹	Retention after 1000 cycles	[3]
a- Ti ₃ C ₂ -T _x	50 mAh g ⁻¹	0.2 A g ⁻¹	Retention after 500 cycles	[4]
c- Ti ₃ C ₂ -T _x	246 mAh g ⁻¹	0.02 A g ⁻¹	Retention after 50 cycles	[5]
TiO ₂ / Ti ₃ C ₂ -T _x	124 mAh g ⁻¹	50 mA g ⁻¹	Retention after 400 cycles	[6]
Ti ₃ C ₂ -F	142 mAh g ⁻¹	50 mA g ⁻¹	89.7% retention after 500 cycles	This work

References:

1. S. J. Kim, N. Michael, Z. Mengqiang, Z. Chuanfang, J. Hee-Tae, W. B. Michel, and G. Yury, *Electrochim. Acta*, 2015, **163**, 246-251.
2. C. Yang, L. Yang, S. Xuan, Z. Yanru, H. Linrui, Z. Qingan, Y. Changzhou *Electrochimica Acta*, 2018, **271**, 165-172.
3. X. Wang, S. Xi, G. Yurui, W. Zhaoxiang, Y. Yu, C. Liquan, *J. Am. Chem. Soc.*, 2015, **137**, 2715-2721.
4. P. Lian, D. Yanfeng, W. Zhong-Shuai, Z. Shuanghao, W. Xiaohui, W. Sen, S. Chenglin, Q. Jieqiong, S. Xiaoyu, B. Xinhe, *Nano Energy*, 2017, **40**, 1-8.
5. V. Natu, C. Mallory, P. Ekaterina, W. B. Michel. *Mater. Res. Lett.*, 2018, **4**, 230-235.
6. C. Zhang, J. K. Seon, G. Michael, Z. Meng-Qiang, W. B. Michel, N. Valeria, G. Yury, *Adv. Funct. Mater.*, 2016, **26**, 4143-4151.