

Supporting Information

MXene Derived-TiO₂/β-Ag₂MoO₄ Nanocomposite: A Multifunctional Electrode for Enhanced Energy Storage in Supercapacitors and Lithium-Ion Batteries

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2.5. Physical Characterization

XRD studies were conducted using Cu K α radiation ($\lambda = 1.5406 \text{ \AA}$, 40 kV, 40 mA) in the 2 θ range of 5-90°. Raman analysis was done by Micro-Raman Spectrometer (LabRAM HR Evolution HORIBA France), using powder samples on a glass substrate. An Oxxius laser of 633 nm wavelength (having a max. power of 100 mW) was used throughout the complete measurement. The morphology and the elemental mapping of the heterostructure were analyzed using high-resolution scanning electron microscopy (HRSEM), Thermo Scientific Apreo instrument operated at an acceleration voltage of 20 kV. Transmission electron microscopy (TEM) images were collected using JEOL Japan, JEM-2100 plus transmission electron microscope operated at an acceleration voltage of 200 kV with the electron source of thermionic LaB₆ single crystal. X-ray photoelectron spectroscopic (XPS) measurements were done with PHI Versaprobe III XPS instrument, and all individual spectra were deconvoluted and fitted using the Shirley-type background function.

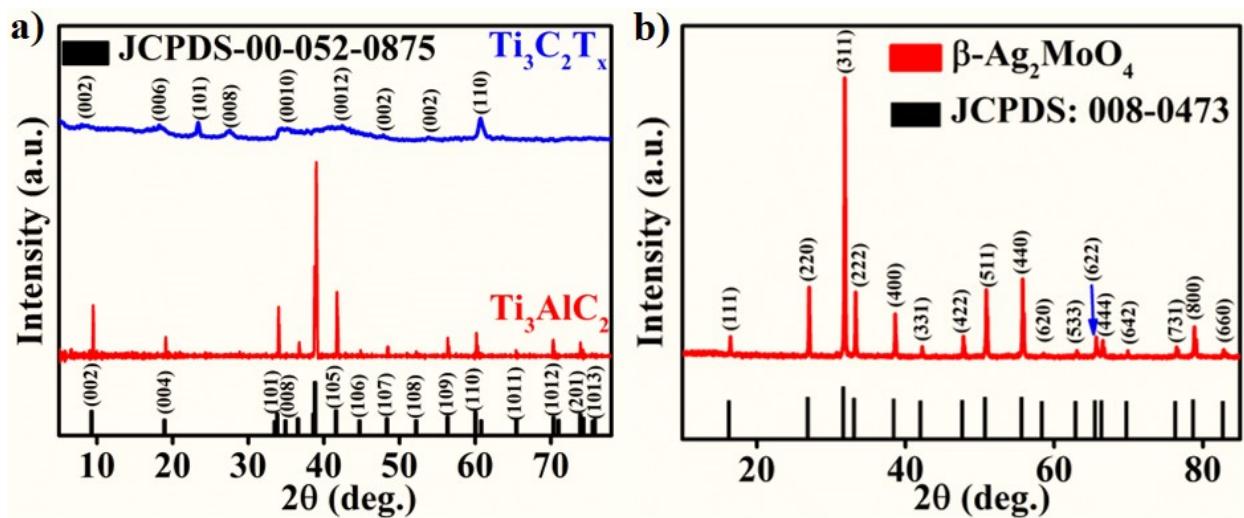


Figure S1. XRD pattern of (a) Ti_3AlC_2 , $\text{Ti}_3\text{C}_2\text{T}_x$ and; (b) $\beta\text{-Ag}_2\text{MoO}_4$.

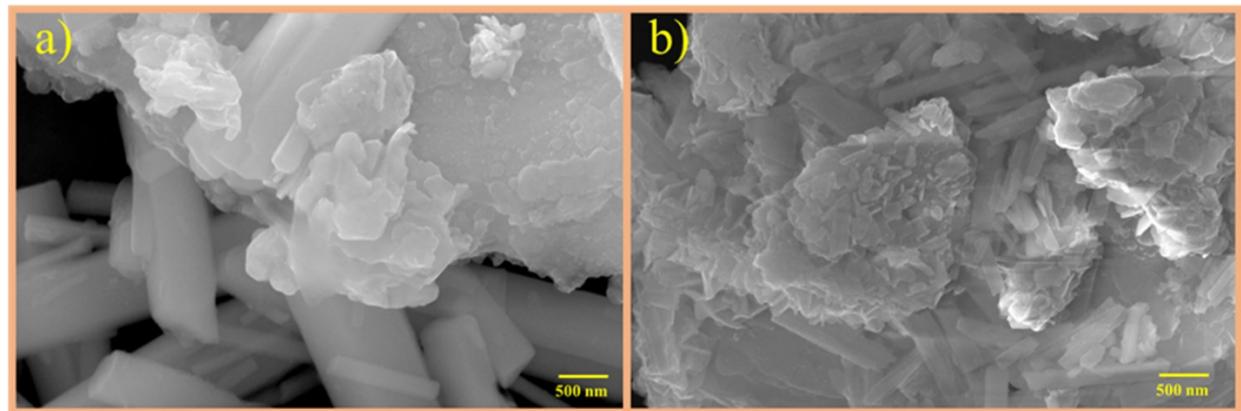


Figure S2. SEM image of (a) $\text{M-TiO}_2/\beta\text{-Ag}_2\text{MoO}_4\text{-1}$ and; (b) $\text{M-TiO}_2/\beta\text{-Ag}_2\text{MoO}_4\text{-3}$ nanocomposite.

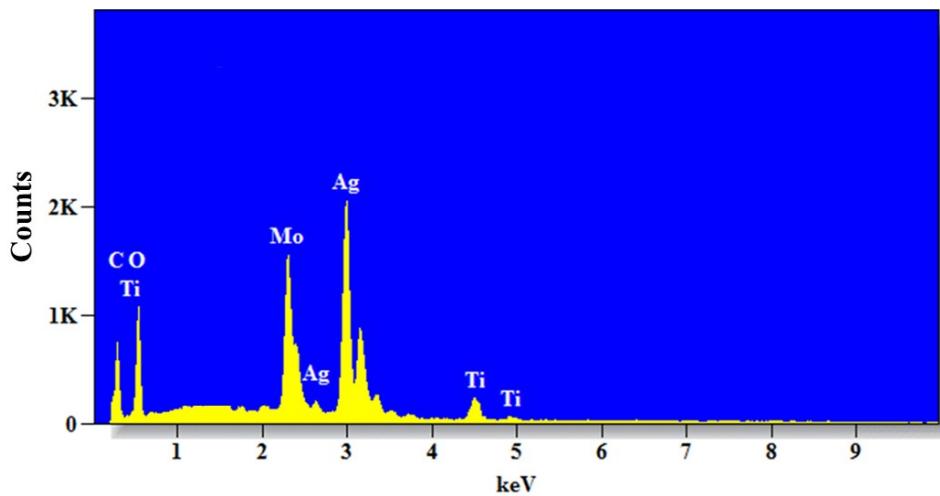


Figure S3. The EDX of M-TiO₂/β-Ag₂MoO₄-2 nanocomposite.

Table S1. Elemental composition of Ti₃C₂T_x, β-Ag₂MoO₄ and M-TiO₂/β-Ag₂MoO₄-2 nanocomposite.

| Materials | Titanium | Silver | Molybdenum | Oxygen | Carbon | Fluorine |
|-----------------------------------------------------------|----------|--------|------------|--------|--------|----------|
| | at% | at% | at% | at% | at% | at% |
| Ti ₃ C ₂ T _x | 53.0 | | | 6.0 | 16.0 | 25.5 |
| β-Ag ₂ MoO ₄ | | 28.6 | 13.9 | 57.5 | | |
| M-TiO ₂ /β-Ag ₂ MoO ₄ -2 | 2.1 | 11.5 | 6.2 | 61.7 | 18.5 | |

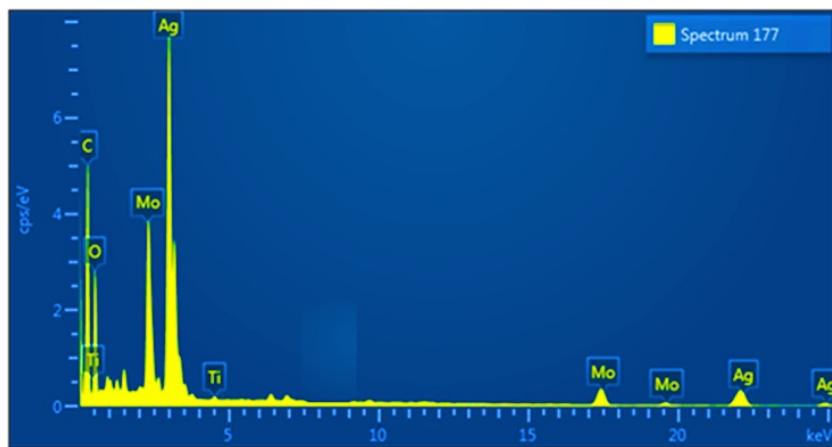


Figure S4. The EDS of M-TiO₂/β-Ag₂MoO₄-2 nanocomposite.

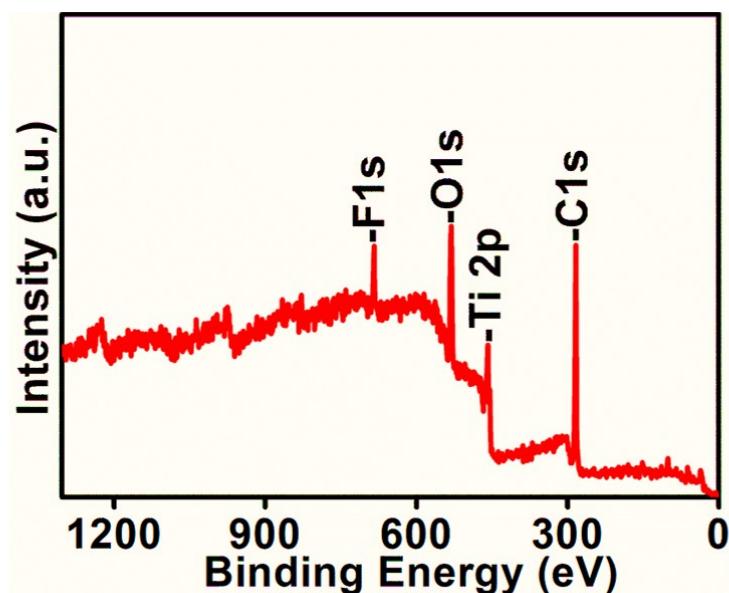


Figure S5. Survey spectrum of MXene (Ti₃C₂T_x).

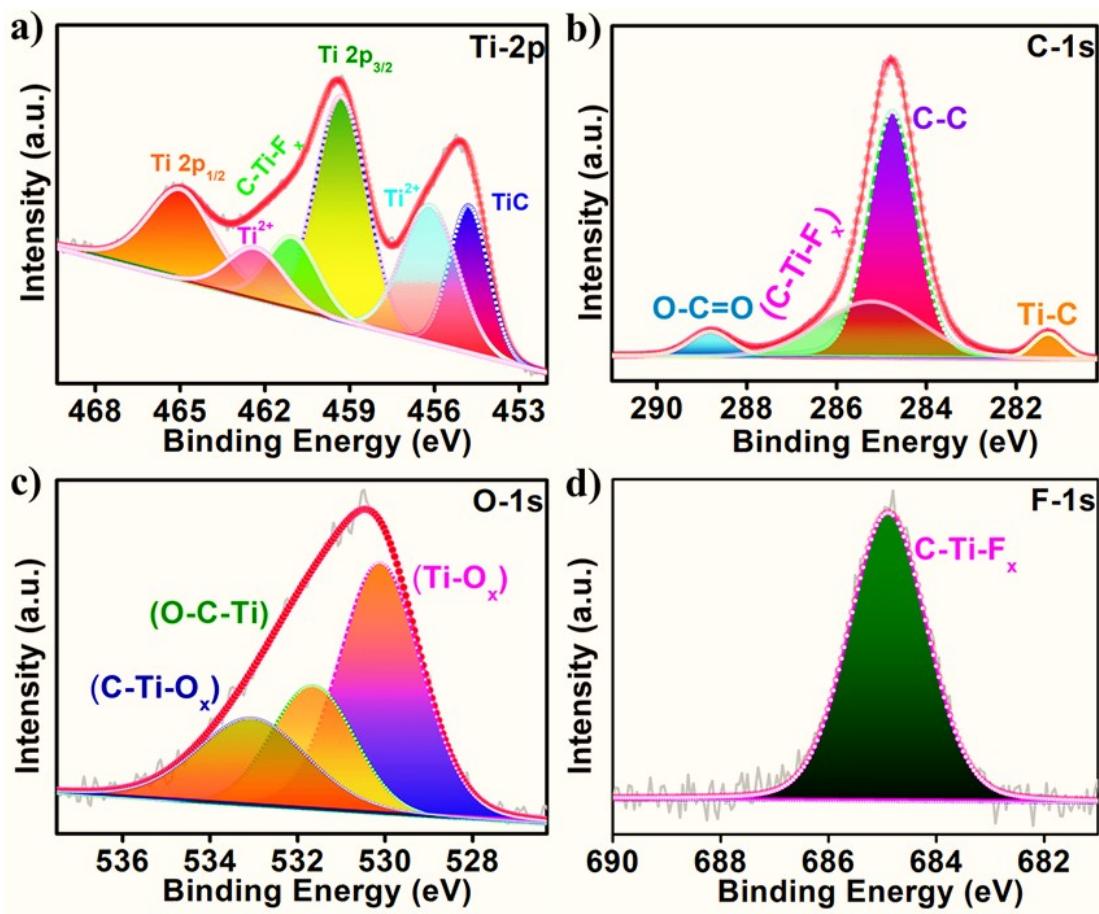


Figure S6. XPS of MXene ($\text{Ti}_3\text{C}_2\text{T}_x$); (a) Ti 2p, (b) C 1s, (c) O 1s, (d) F 1s.

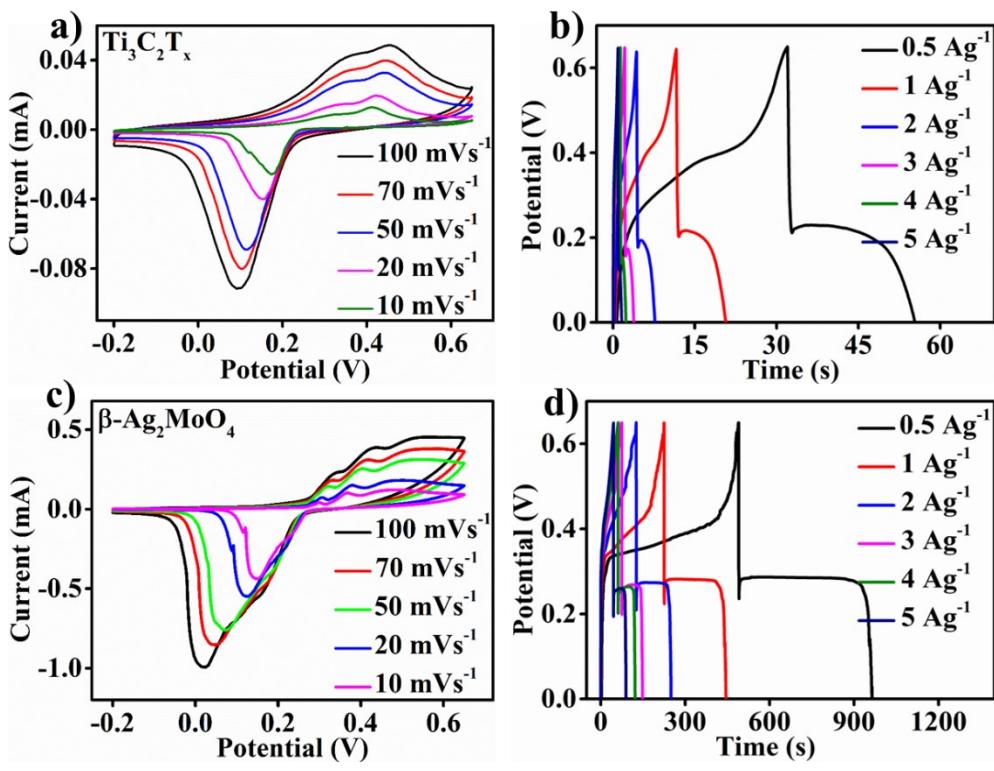


Figure S7. (a, c) CV curves at various scan rate and; (b, d) GCD profiles at different current density of $\text{Ti}_3\text{C}_2\text{T}_x$ and $\beta\text{-Ag}_2\text{MoO}_4$.

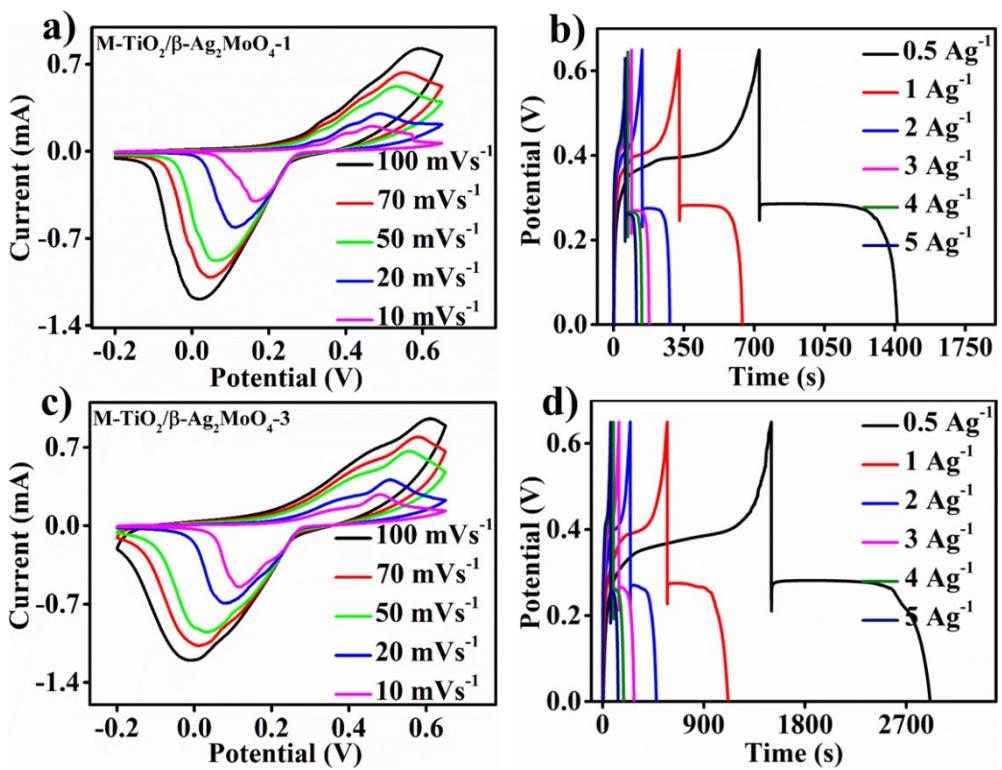


Figure S8. (a, c) CV curves at various scan rate and; (b, d) GCD profiles at different current density of $\text{M-TiO}_2/\beta\text{-Ag}_2\text{MoO}_4\text{-1}$ and $\text{M-TiO}_2/\beta\text{-Ag}_2\text{MoO}_4\text{-3}$ nanocomposite.

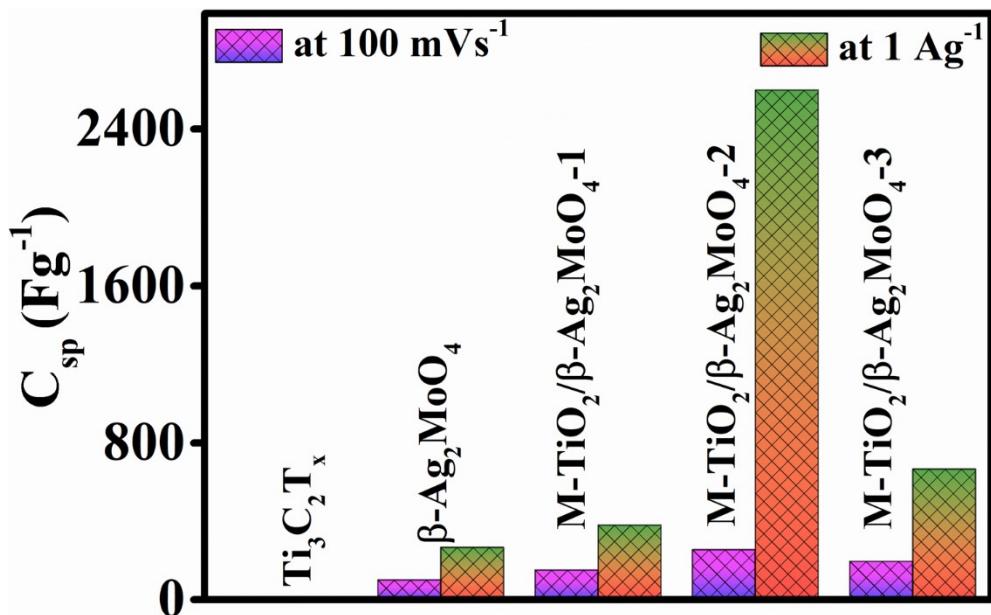


Figure S9. The calculated specific capacitance in three electrode configurations for various active electrode materials at 100 mV s^{-1} and 1 A g^{-1} .

Table S2. The calculated specific capacitance in three electrode configurations for various active electrode materials.

| Materials | Specific capacitance (F g^{-1}) | |
|---------------------------------------------------------|--------------------------------------------|-------------------------------|
| | by CV @ 100 mV s^{-1} | by GCD @ 1 A g^{-1} |
| $\text{Ti}_3\text{C}_2\text{T}_x$ | 11.8 | 12.1 |
| $\beta\text{-Ag}_2\text{MoO}_4$ | 100.8 | 266.6 |
| $\text{M-TiO}_2/\beta\text{-Ag}_2\text{MoO}_4\text{-1}$ | 151.4 | 380.0 |
| $\text{M-TiO}_2/\beta\text{-Ag}_2\text{MoO}_4\text{-2}$ | 255.8 | 2599 |
| $\text{M-TiO}_2/\beta\text{-Ag}_2\text{MoO}_4\text{-3}$ | 195.4 | 666.2 |

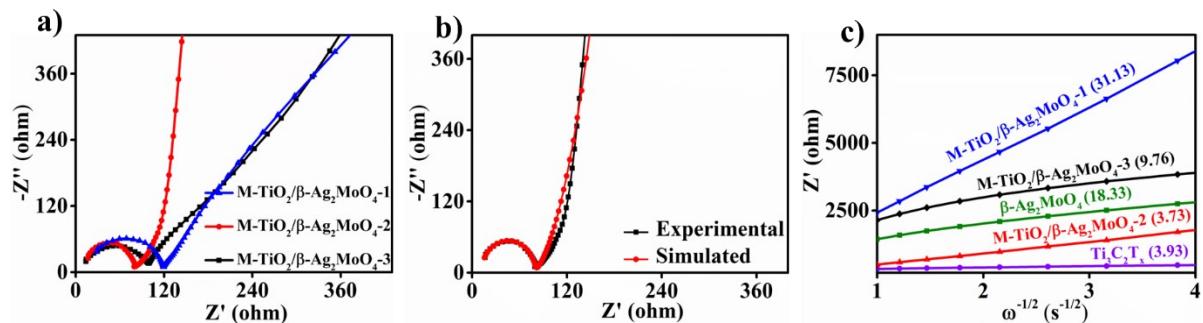


Figure S10. (a) Nyquist plots of all nanocomposites; (b) Experimental and fitted EIS curve for M-TiO₂/β-Ag₂MoO₄-2 electrode; (c) Plot of Z' versus reciprocal square root of frequency ($\omega^{-1/2}$).

Table S3. The transport properties of various electrodes were obtained from simulated impedance spectra in Fig. (5f)

| Electrode | R _s (Ω) | R _{ct} (Ω) | σ = (Ω s ^{-1/2}) | C _{ad} (mF) |
|-----------------------------------------------------------|--------------------|---------------------|----------------------------|----------------------|
| Ti ₃ C ₂ T _x | 14.4 | 113.8 | 3.93 | 5.6 |
| β-Ag ₂ MoO ₄ | 31.8 | 119.2 | 18.33 | 1.7 |
| M-TiO ₂ /β-Ag ₂ MoO ₄ -1 | 28.1 | 116.8 | 31.13 | 0.07 |
| M-TiO ₂ /β-Ag ₂ MoO ₄ -2 | 16.4 | 82.3 | 3.73 | 0.03 |
| M-TiO ₂ /β-Ag ₂ MoO ₄ -3 | 13.8 | 99.1 | 9.76 | 0.05 |

Table S4. The calculated specific capacitance of M-TiO₂/β-Ag₂MoO₄-2 electrode material under the three-electrode configuration.

| Cycles No. | Specific Capacitance (F g ⁻¹) | |
|------------|-------------------------------------------|------------------------------|
| | by CV @ 100 mV s ⁻¹ | by GCD @ 1 A g ⁻¹ |
| 0k | 255.8 | 2599 |
| 5k | 198.5 | 2600 |
| 10k | 208.7 | 2584 |
| 15k | 209.8 | 2626 |
| 20k | 204.7 | 2614 |
| 25k | 195.5 | 2565 |

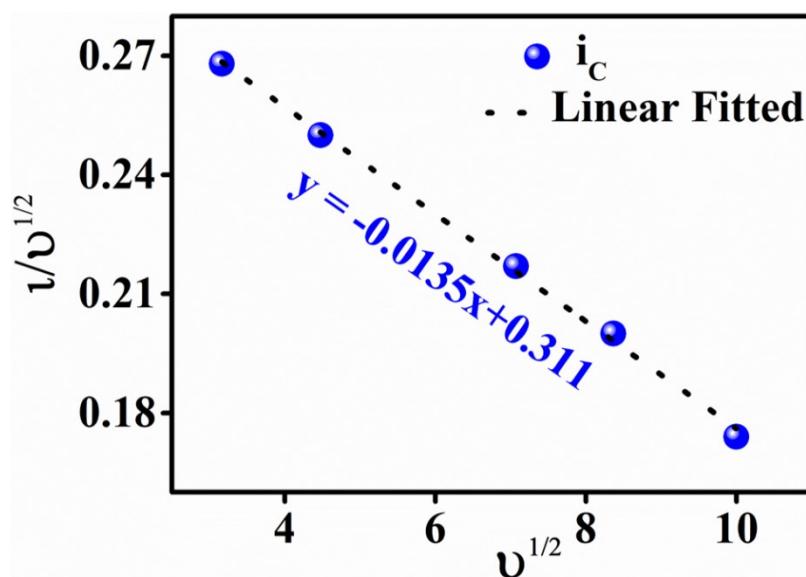


Figure S11. Plot of $i/(v)$ against $v^{0.5}$ for the cathodic sweeps under an alkaline medium to evaluate the value of k_1 and k_2 in the equation 12 and 13.

Table S5. The capacitive and diffusion contribution was calculated by the Dunn Method

| v | $v^{1/2}$ | i | k_1 | k_2 | k_1v | $k_2v^{1/2}$ | $k_1v+k_2v^{1/2}$ | $k_1v/i(v) = \frac{k_1v + k_2v^{1/2} * 100}{k_1v + k_2v^{1/2} * 100 - 100}$ | $\frac{k_2v/i(v)}{k_1v + k_2v^{1/2} * 100 - 100}$ | Toal capacity | $k_1v\ %$ | $k_2v^{1/2}\ %$ |
|-----|-----------|------|--------|-------|--------|--------------|-------------------|-----------------------------------------------------------------------------|---------------------------------------------------|---------------|-----------|-----------------|
| 10 | 3.162 | 0.86 | 0.0135 | 0.311 | 0.135 | 0.983382 | 1.118382 | 12.07100973 | 87.92899027 | 1218 | 146 | 1072 |
| 20 | 4.472 | 1.12 | 0.0135 | 0.311 | 0.27 | 1.390792 | 1.660792 | 16.25730374 | 83.74269626 | 811 | 130 | 681 |
| 50 | 7.071 | 1.54 | 0.0135 | 0.311 | 0.675 | 2.199081 | 2.874081 | 23.48576815 | 76.51423185 | 439 | 101 | 339 |
| 70 | 8.366 | 1.67 | 0.0135 | 0.311 | 0.945 | 2.601826 | 3.546826 | 26.64353989 | 73.35646011 | 343 | 92 | 251 |
| 100 | 10 | 1.74 | 0.0135 | 0.311 | 1.35 | 3.11 | 4.46 | 30.2690583 | 69.7309417 | 178 | 77 | 178 |

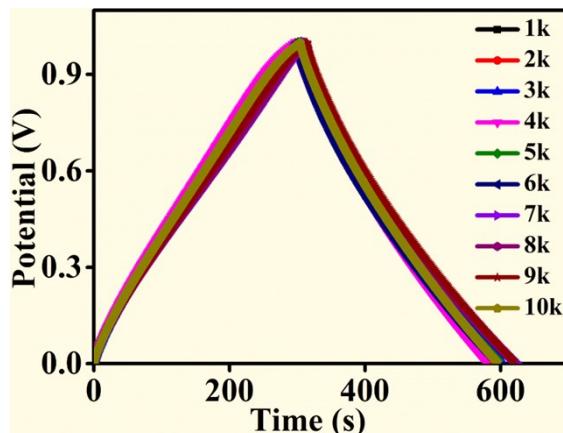


Figure S12. GCD curves at 1 A g^{-1} up to 10,000 cycles.

Table S6. The calculated specific capacitance on GCD curve of the as-fabricated symmetric coin cell supercapacitor throughout the stability performance.

| Cycles No. | Specific Capacitance (F g^{-1}) |
|------------|--------------------------------------------|
| | by GCD @ 1 A g^{-1} |
| 1k | 292.8 |
| 2k | 285.0 |
| 3k | 297.2 |
| 4k | 283.4 |
| 5k | 295.7 |
| 6k | 290.2 |
| 7k | 310.2 |
| 8k | 309.0 |
| 9k | 305.2 |
| 10k | 290.4 |

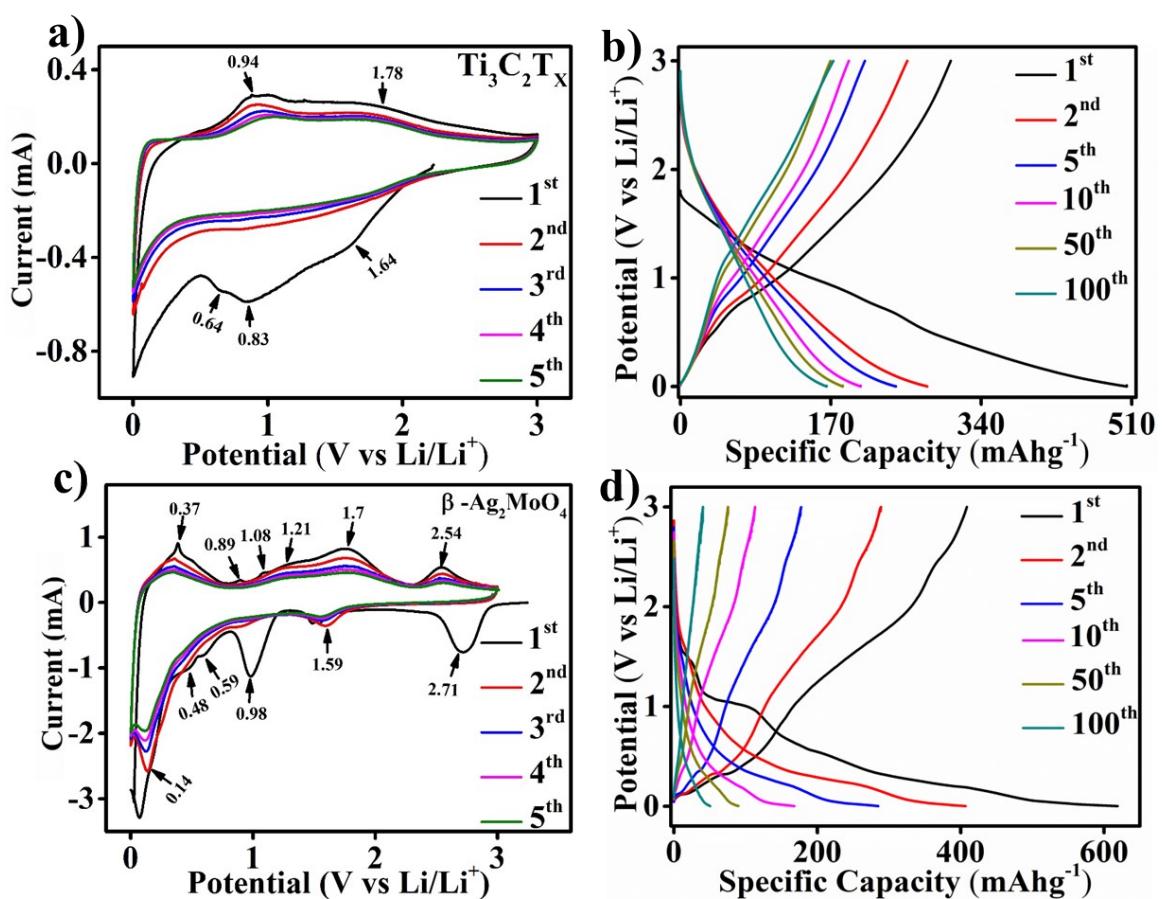


Figure S13. (a, c) CV of the MXene, $\beta\text{-Ag}_2\text{MoO}_4$ at 0.2 mV s^{-1} scan rate; (b, d) GCD curves of MXene, $\beta\text{-Ag}_2\text{MoO}_4$ at current density of 100 mA g^{-1} .

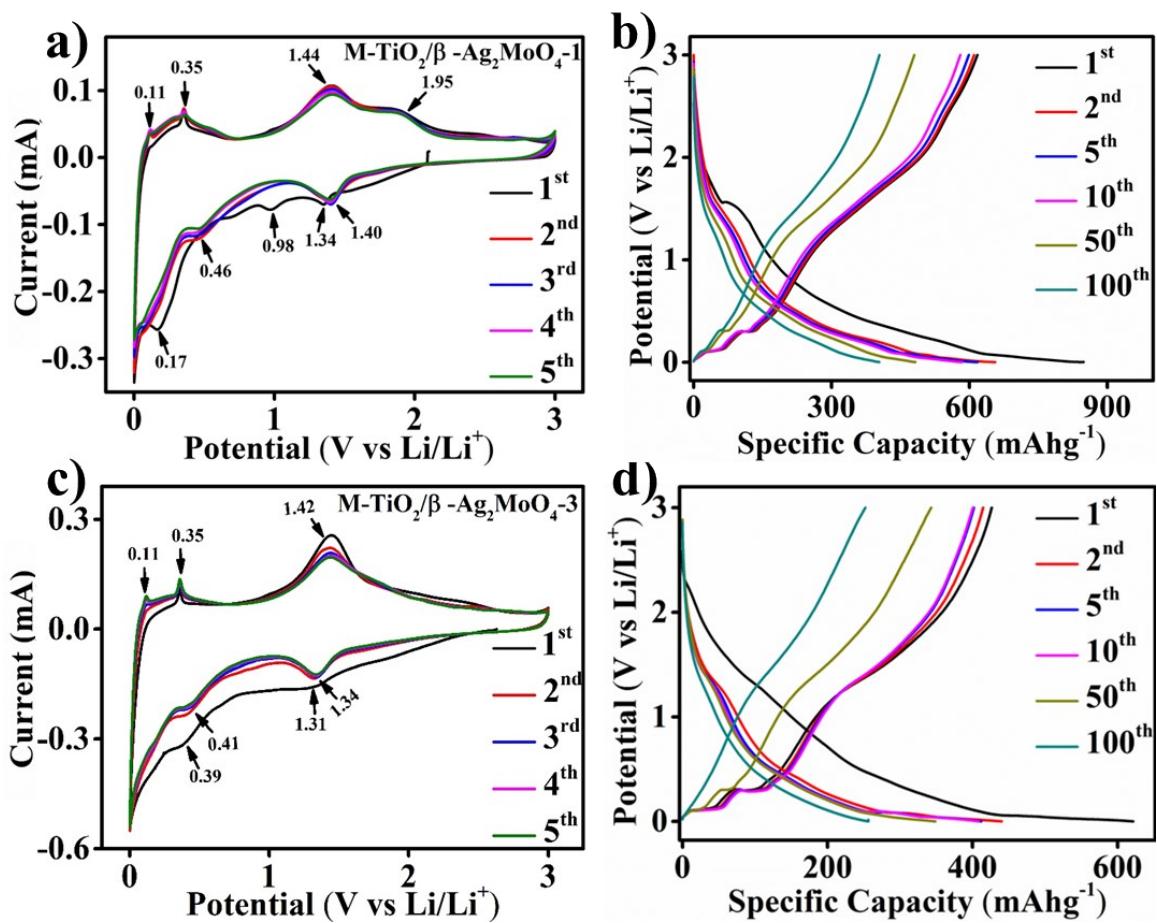


Figure S14. (a, c) CV of the $\text{M-TiO}_2/\beta\text{-Ag}_2\text{MoO}_4\text{-1}$ and $\text{M-TiO}_2/\beta\text{-Ag}_2\text{MoO}_4\text{-3}$ at 0.2 mV s^{-1} scan rate; (b, d) GCD curves of $\text{M-TiO}_2/\beta\text{-Ag}_2\text{MoO}_4\text{-1}$ and $\text{M-TiO}_2/\beta\text{-Ag}_2\text{MoO}_4\text{-3}$ at current density of 100 mA g^{-1} .

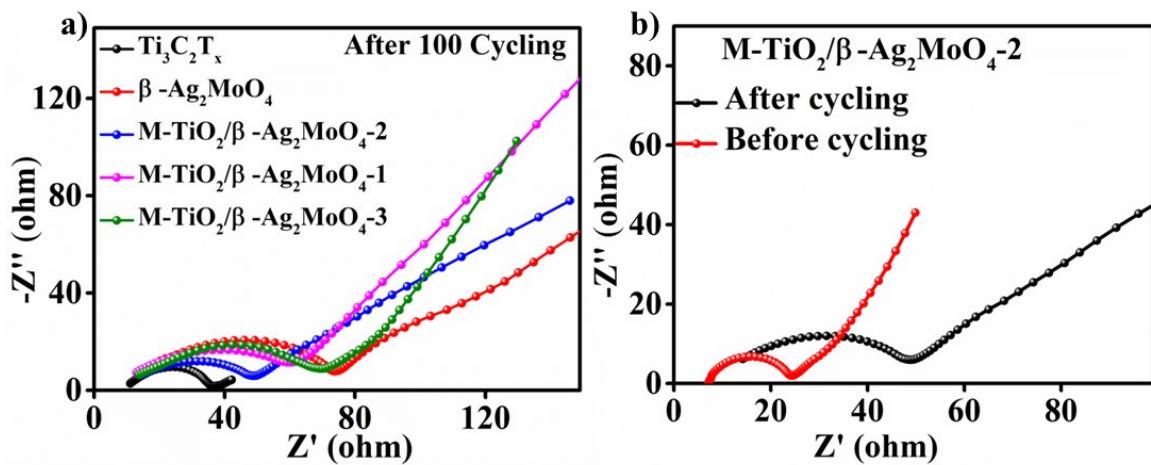


Figure S15. (a) EIS curve for MXene, β -Ag₂MoO₄ and all synthesized nanocomposites in the 0.1 Hz to 10 kHz frequency range. (b) Nyquist plot of after and before cycling stability of M-TiO₂/ β -Ag₂MoO₄-2 nanocomposite.

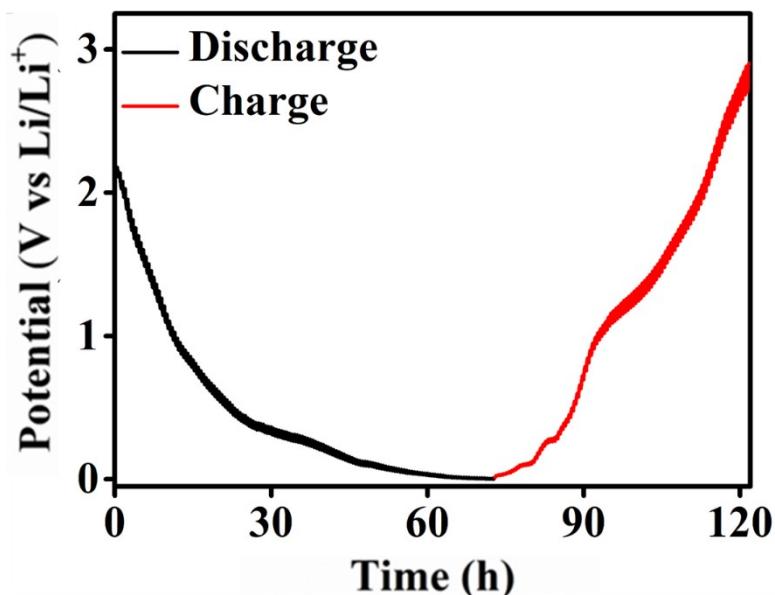


Figure S16. Galvanostatic intermittent titration technique (GITT) study of the M-TiO₂/ β -Ag₂MoO₄-2 working electrode.

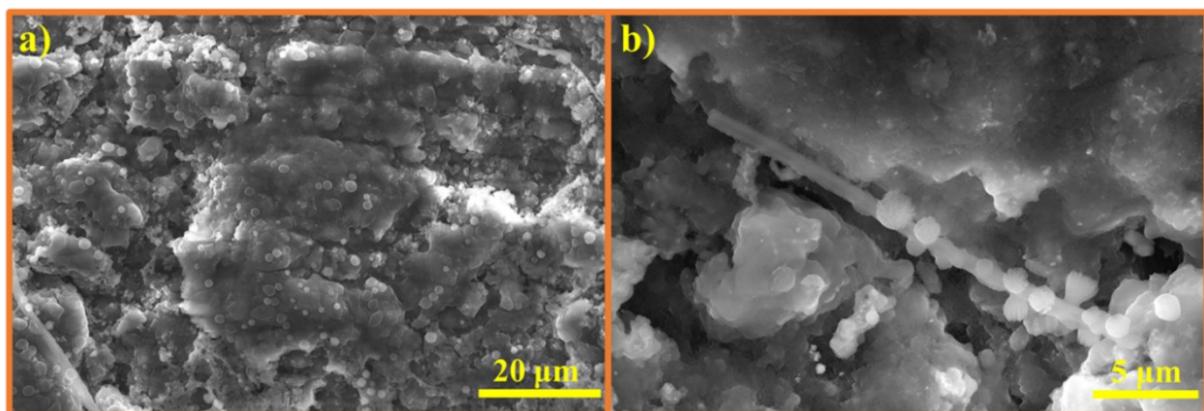


Figure S17. (a, b) HRSEM cross-section morphology of M-TiO₂/β-Ag₂MoO₄-2 working electrode after 100 cycles charge-discharge curve.

Table S7. The comparative electrochemical performance of the MXene and binary metal oxide-based electrode material for supercapacitor.

| Materials | Preparation Method | Electrolyte [Mol L ⁻¹] | Specific Capacitance | | Cycling Stability 3E (a) | Cycling Stability 2E (b) | Ref. |
|------------------------------------------------------------------|----------------------------|---------------------------------------|--------------------------------------------------|---------------|--------------------------|--------------------------|------|
| | | | Electrode 3E (a) | Device 2E (b) | | | |
| NiCo ₂ O ₄ @Fe ₂ O ₃ | Hydrothermal & Calcination | 1.0 M Na ₂ SO ₄ | 262 mF cm ⁻² at 1 mA cm ⁻² | ---- | 74.2 % @4000 | ---- | 1 |

| | | | | | | | |
|-------------------------------------------------------------------------------------|----------------------------------|----------------------------------------|--------------------------------------------------------|-------------------------------------------------------|--------------------------|--------------------------|----------------------|
| NiO/ NiMoO ₄ | Reflux & Calcination | 6.0 M KOH | 1624.5 F g ⁻¹ at 1.0 A g ⁻¹ | ---- | 73.5 % @2200 | ---- | 2 |
| NiCo ₂ O ₄ @ rGO/ACF | Hydrothermal & Calcination | 3 M KOH | 1338 mF cm ⁻² at 3 mA cm ⁻² | ---- | 88.2 % @10 000 | ---- | 3 |
| NiMoO ₄ / Ti ₃ C ₂ T _x -10 | Annealing | 3 M KOH | 483.8 C g ⁻¹ at 1.0 A g ⁻¹ | ---- | 68.0 % @10 000 | ---- | 4 |
| NiZnCoO ₄ / CoWO ₄ -10 | Hydrothermal & Calcination | 2 M KOH | 370.9 F g ⁻¹ at 0.5 A g ⁻¹ | ---- | 90 % @500 | ---- | 5 |
| MnCo ₂ O _{4.5} @NiCo ₂ O ₄ | Hydrothermal & Calcination | 3 M KOH | 325 F g ⁻¹ at 1 A g ⁻¹ | ---- | 70.5 % @ 3000 | ---- | 6 |
| ZnFe ₂ O ₄ - rGO | Hydrothermal | 2 M KOH | 1419 F g ⁻¹ at 100 mV s ⁻¹ | 101 F g ⁻¹ at 0.5 A g ⁻¹ | 93 % @5000 | 90.1 % @5000 | 7 |
| Ti ₃ C ₂ T _x /M nCo ₂ O ₄ | Hydrothermal & Calcination | 1 M KOH | 806.6 F g ⁻¹ at 1 A g ⁻¹ | ---- | 77 % @3000 | ---- | 8 |
| MoO ₃ /Ti ₃ C ₂ T _x | Hydrothermal | 1 M KOH | 151 F g ⁻¹ at 2 mV s ⁻¹ | ---- | 93.7 % @8000 | ---- | 9 |
| Ti ₃ C ₂ T _x /α- MoO ₃ | Hydrothermal | 1 M Na ₂ SO ₄ | 371 C g ⁻¹ at 1.0 A g ⁻¹ | ---- | 89.5 % @6000 | ---- | 10 |
| β- Ag ₂ MoO ₄ | Rapid wet chemical method | 2 M KOH | 2610 C g ⁻¹ at 1 A g ⁻¹ | ---- | 82 % @5000 | ---- | 11 |
| Ti ₃ C ₂ T _x /Ag ₂ CrO ₄ | co- precipitation method | 0.1M H ₂ SO ₄ | 525 F g ⁻¹ at 10 mV s ⁻¹ | ---- | ---- | ---- | 12 |
| Ti ₃ C ₂ T _x /CuCr ₂ O ₄ | co- precipitation method | 0.1M H ₂ SO ₄ | 445.5 F g ⁻¹ at 20 mV s ⁻¹ | ---- | ---- | ---- | 13 |
| M-TiO ₂ /β- Ag ₂ MoO ₄ - 2 | Reflux method | 0.1 M KOH | 2599 F g⁻¹ at 1 A g⁻¹ | 309 F g⁻¹ at 1 A g⁻¹ | 98.7 % @25000 | 95.1 % @10000 | This Work |

Table S8. The comparative electrochemical performance of the MXene and binary metal oxide-based electrode material for Lithium-ion Battery.

| Materials | Preparation Method | Initial discharge capacity (mA hg ⁻¹) | Capacity (mA hg ⁻¹)/ Cycles (times) @ current density mA g ⁻¹ | Ref. |
|------------------------------------------------|-----------------------|------------------------------------------------------|--------------------------------------------------------------------------------------------|---------------|
| C-Li ₂ MoO ₄ nanotube | Sol-gel method | ~ 650 mA hg ⁻¹ | ~ 550 mA hg ⁻¹ /23@90 mA g ⁻¹ | ¹⁴ |

| | | | | |
|-----------------------------------------------------------------------------|----------------------|--------------------------------|---------------------------------------------------------|------------------|
| MoO ₃ /C | Electro-spinning | 1550 mA hg ⁻¹ | 710 mA hg ⁻¹ /100 @40 mA g ⁻¹ | 15 |
| h-MoO ₃ | Reflux | 1869 mA hg ⁻¹ | 619 mA hg ⁻¹ /100@C/15 | 16 |
| C-coated α -Na ₂ MoO ₄ nanoplate | Sol-gel method | 806 mA hg ⁻¹ | 320 mA hg ⁻¹ /50@30 mA g ⁻¹ | 17 |
| MXene/Ag | Conventional method | 550 mA hg ⁻¹ | 310 mA hg ⁻¹ /800@1C | 18 |
| M-TiO₂/β-Ag₂MoO₄-2 | Reflux method | 1013 mA hg⁻¹ | 335 mA hg⁻¹/100@100 mA g⁻¹ | This work |

Table S9. The transport properties of various electrodes were obtained from impedance spectra in Fig S15.(a)

| Electrode | R _s (Ω) | R _{ct} (Ω) |
|-------------------------------------------------------------------|-----------------------------|------------------------------|
| Ti ₃ C ₂ T _x | 12.1 | 36.0 |
| β -Ag ₂ MoO ₄ | 20.6 | 73.5 |
| M-TiO ₂ / β -Ag ₂ MoO ₄ -1 | 13.5 | 60.4 |
| M-TiO ₂ / β -Ag ₂ MoO ₄ -2 | 15.1 | 47.9 |
| M-TiO ₂ / β -Ag ₂ MoO ₄ -3 | 16.1 | 68.6 |

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