Supporting Information

High-power two-dimensional molybdenum boride MBene electrodes for lithium-ion batteries and capacitors

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Table S1. Elemental composition of $Mo_{4/3}Y_{2/3}AlB_2$ *i*-MAB phase and $Mo_{4/3}B_2T_x$ *i*-MBene aerogel as determined by energy dispersive spectroscopy (EDS).

	$Mo_{4/3}Y_{2/3}AlB_2$ *i*-MAB phase		$Mo_{4/3}B_2T_x$ *i*-MBene aerogel	
Element	at%	Ratio to $Mo_{4/3}$	at%	Ratio to $Mo_{4/3}$
Mo	16.94	1.33	12.3	1.33
Y	9.04	0.71	0.97	0.10
Al	16.16	1.27	0.72	0.08

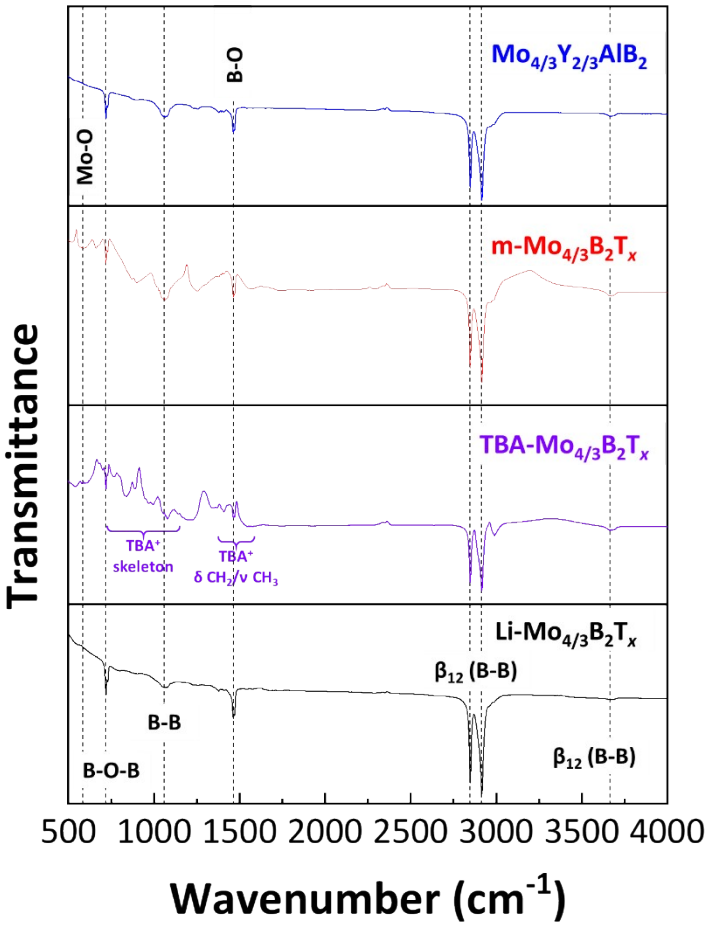

Figure S1. ATR-FTIR spectra for $Mo_{4/3}Y_{2/3}AlB_2$, $Mo_{4/3}B_2T_x$ *i*-MBene multilayered, TBAOH delaminated $Mo_{4/3}B_2T_x$ aerogel and LiCl treated $Mo_{4/3}B_2T_x$ aerogel.

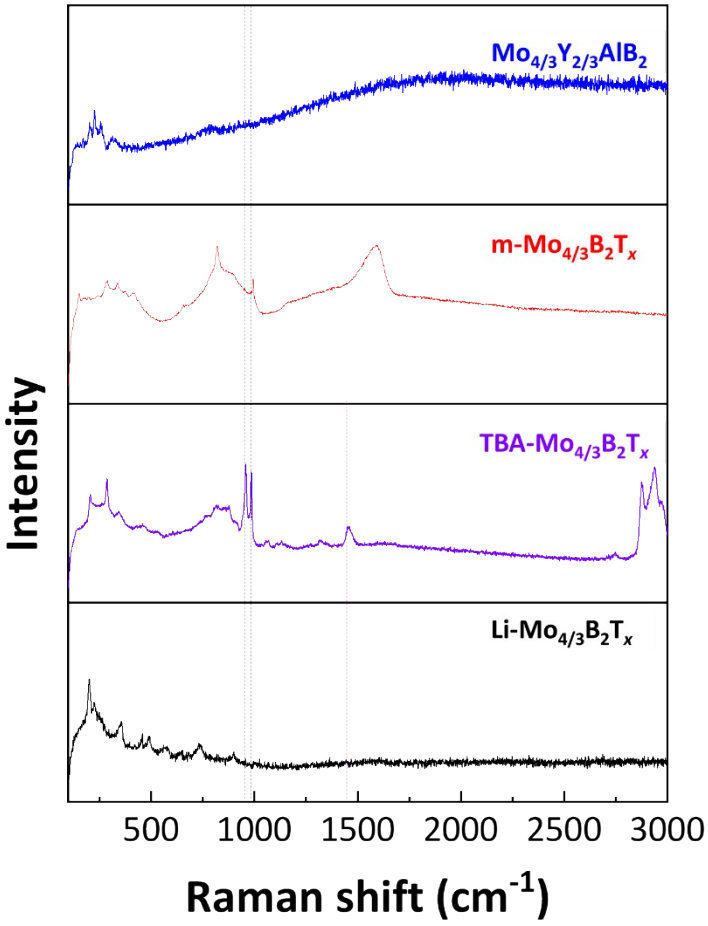

Figure S2. Raman spectra for $Mo_{4/3}Y_{2/3}AlB_2$, $Mo_{4/3}B_2T_x$ *i*-MBene multilayered, TBAOH delaminated $Mo_{4/3}B_2T_x$ aerogel and LiCl treated $Mo_{4/3}B_2T_x$ aerogel.

Table S2. Calculated lattice parameters for Li bulk and $Mo_{4/3}B_2$ and comparison to previous calculations.

Parameter	Value (Å)	Reference
Li bulk lattice constant	3.439	Our calculation
Li bulk lattice constant	3.451	[1]
$Mo_{4/3}B_2$ lattice constant	5.172	Our calculation
$Mo_{4/3}B_2$ lattice constant	5.170	[2]

Table S3. Li intercalation energy values for $Mo_{4/3}B_2O_2$.

Parameter	Energy (eV)	How the value was obtained
Li diffusion barrier	0.447	$\lvert E_{hexagon} - E_{TS} \rvert$
Li bridge site V1 adsorption energy	-2.507	$E_{surf+Li} - E_{Li} - E_{surf}$
Li bridge site V2 adsorption energy	-2.574	$E_{surf+Li} - E_{Li} - E_{surf}$
Li top site adsorption energy	-1.949	$E_{surf+Li} - E_{Li} - E_{surf}$
Li hexagon adsorption energy	-2.738	$E_{surf+Li} - E_{Li} - E_{surf}$
Li transition state (TS)	-2.292	$E_{surf+Li} - E_{Li} - E_{surf}$

Table S4. Equivalent circuit fitting of PEIS analysis of Mo_2AlB_2 and $Mo_{4/3}B_2T_x$.

	ESR (Ω)	**R_{CT} (Ω)**	**Q_{DL} ($F \cdot s^{(n-1)}$)**	**n_{DL}**	**Q_{LF} ($F \cdot s^{(n-1)}$)**	**n_{LF}**	**M_α (Ω)**	**τ_D (s)**	**α**
$Mo_{1.33}B_2T_x$	9.5	168.4	$3.9 \cdot 10^{-5}$	0.702	$3.5 \cdot 10^{-3}$	0.591	243	1.8	0.746
	ESR (Ω)	**R_{CT} (Ω)**	**Q_{DL} ($F \cdot s^{(n-1)}$)**	**n_{DL}**	**Q_{LF} ($F \cdot s^{(n-1)}$)**	**n_{LF}**	**M_γ (Ω)**	**τ_D (s)**	**γ**
Mo_2AlB_2	6.2	29.2	$4.1 \cdot 10^{-5}$	0.760	$8.4 \cdot 10^{-4}$	0.323	524	0.8	0.185

References

1. P. Haas, F. Tran and P. Blaha, *Physical Review B*, 2009, **79**.
2. P. Helmer, J. Halim, J. Zhou, R. Mohan, B. Wickman, J. Björk and J. Rosen, *Advanced Functional Materials*, 2022, **32**.