Designing Effective Solvent–Catalyst Interface for Catalytic Sulfur Conversion in Lithium–Sulfur Batteries

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Additional Experimental Section

Materials Characterizations.

The Brunauer-Emmett-Teller (BET) surface area was measured using a Micromeritics ASAP 2020 Surface Area and Porosity Analyzer.

S L-edge XANES for soaked material powders were obtained at the Canadian Light Source (CLS) on the VLS-PGM beamline. All the samples were stored in argon and transferred through an argon-filled glove box into the connected vacuum chamber of beamline's Endstation. Spectra were collected under TEY mode providing surface information with the depth of ~10 nm. XANES spectra were normalized by the I₀ current, which was collected by a Nickel mesh placed in front of sample. Origin (OriginLab) was used to process the spectra. Preparation of the powder sample with same total surface area (i.e., TiX powder and Vulcan XC-72 carbon with specific surface area of 218 m² g⁻¹, Cobot Co., USA) was the same as that for XPS measurement. Cathode interlayer sample in DMSO-based Li-S batteries for exsitu XANES measurement were prepared with 1.0 M LiClO₄-0.4 M LiNO₃ in DMSO as the electrolyte which were found not influence the galvanostatic behavior of Li-S batteries in the first few cycles. The interlayer samples were collected at certain stages from the DMSO-based Li-S batteries with sulfur loading of 2 mg_s cm⁻² under 0.02 C, and washed with DMSO pure solvent to remove extra supporting salts and free polysulfide species. All the XANES samples were vacuum dried before transforming to the testing chamber.

X-ray diffraction (XRD) XRD results of commercial TiB₂, TiC and TiO₂ powders were collected using a Rigaku SmartLab diffractometer (Cu K α radiation) with a continuous scan of 5° min⁻¹ between 2 θ from 10° to 90°.

Scanning electron microscope (SEM) and Transmission electron microscope (TEM) The particle sizes of TiB₂, TiC and TiO₂ nano powders used in this work were analyzed using SEM on Quanta 400 FEI scanning electron microscope and bright field TEM on FEI Tecnai G2 Spirit Twin TEM, respectively. Samples for TEM tests were prepared after sonication the nano powder in ethanol and loaded onto a Cu grid.

Electrochemical measurements.

One compartment Li-S batteries (Figure S9a) Electrochemical impedance spectroscopy (EIS) measurements for routine loading cell were conducted before all tests on Bio-Logic VMP3 with the oscillation frequency range from 1 MHz to 100 mHz under the sinusoidal voltage oscillations of 5.0 mV amplitude at the open-circuit potential. All of the measurements were scanned with three repetitions.

The sulfur loading for high-energy Li-S batteries were controlled to $5.6 \text{ mg}_{\text{s}} \text{ cm}^{-2}$ on $\Phi 10 \text{ mm}$ graphite felt (Yi Deshang Carbon Technology Co., Ltd.) with the thickness of 0.5 mm. In CR2025 coin cell, the cathode electrode was followed by a TiX functional carbon paper interlayer. One layer of Celgard 2325 was used as the separator and a lithium foil was used as the anode. A gasket and a spring were utilized to guarantee good electronic conductivity between the coin cell case and electrodes. The galvanostatic tests were conducted with the voltage cutoff of 1.7 V for discharge and 3.0 V for charge process, respectively. Electrolyte/sulfur (E/S) ratio was set to 13.6 mL g⁻¹ for high-loading cell.

Two-compartment Li-S batteries (Figure S9b) Galvanostatic charge/discharge curves of Li-S batteries with LAGP as the solid-state electrolyte were measured using a multichannel battery testing system (LAND, CT2001A, Wuhan LAND electronics Co., Ltd.) in a voltage window of 1.6-3.0 V for DOL: DME electrolyte system, and 1.6-3.2 V for DMSO electrolyte system. Bulk sulfur electrode with ~1.1 mg_s cm⁻² loading was employed as the cathode with an interlayer with various TiX materials (0.1 m² per piece).



Figure S1. (a) BET results for specific surface area determination of TiB₂, TiC and TiO₂ used in this work; Barrett–Joyner–Halenda (BJH) desorption pore size distribution of (b) TiB₂, (c) TiC and (d) TiO₂, inset: adsorption/desorption isotherm.

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	BET surface area [m ² g ⁻¹]	BJH desorption cumulative volume of pores [cm ³ g ⁻¹]	BJH desorption average pore diameter [nm]
Titanium diboride (TiB ₂)	28.75	0.053	11.59
Titanium carbide (TiC)	19.03	0.074	21.50
Titanium oxide (TiO ₂)	89.23	0.37	12.07



Figure S2. UV-Vis spectra of TiX powders after soaking in mid- and short- chain polysulfides. (a) TiB₂, TiO₂ soaked in 1.0 mM Li₂S₆ in DOL: DME; (b) TiB₂, TiO₂ soaked in 1.0 mM Li₂S₄ in DOL: DME; (c) TiB₂, TiO₂ soaked in 1.0 mM Li₂S₆ in DMSO; (d) TiB₂, TiO₂ soaked 1.0 mM Li₂S₄ in DMSO.



Figure S3. S L-edge X-ray adsorption spectra (XANES) of the powders (TiX, X=B, C, O and Vulcan XC-72 carbon) retrieved after soaking in Li_2S_8 in (a) DOL: DME and (b) DMSO; (c) S L-edge spectra for various reference samples under FY mode. The spectra of MoS₂ is obtained from Chen et al.¹ The intensity of the TiB₂ spectra is reduced by 2 times and 10 times in DOL:DME and DMSO, respectively.

Notes of S L-edge XANES of catalyst powder after adsorption:

We exploited S L-edge XANES to examine the changes in electronic structure of sulfur after polysulfide adsorption onto the Tibased compounds, providing more sensitive information of sulfur local bonding environment than K-edge due to the well-resolved fine features induced by spin-orbit coupling of S $2p_{3/2}$ and $2p_{1/2}$ electrons.² First, consistent with UV-vis spectra and XPS, TiO₂ shows no obvious L-edge XANES features of sulfur (photon energy: 162 eV (white line) ~ 170 eV) after soaking in both solvents, ¹⁻ ³ confirming that no polysulfide was chemically trapped by TiO₂. In contrast, the XANES intensity of S on TiB₂ is two times that of TiC in DOL: DME, and 10 times that of TiC in DMSO, confirming the strongest polysulfide adsorption abilities of TiB₂ among all three Ti-based materials in both polar and non-polar solvents. The S L-edge features on TiB₂/TiC in DOL:DME shown in Figure S3a can be de-convoluted into three features i.e. **a**, **b** and **c**, which resembles the trigonal prismatic coordination¹. The energy separation of **b** and **c** is 1.2 ± 0.1 eV (Table S2), which is in good agreement with the spin-orbit coupling of S 2p electrons (Figure S3c).² Interestingly, the separation of peak **a** with peak **b** (or **c**) (denoted as ΔE (E2-E1) in Table S2) is decreased with increasing electronegativity of the non-metal elements (from B, C to O), indicating that the non-metal element manipulates the final hybridization orbitals in the newly formed S-Ti-X complex (Figure S3a). In DMSO (Figure S3b and Table S3), quadra-peak shape of XANES spectra were observed in TiB₂ with two sets of peaks with separation of 1.2 ± 0.1 eV (S $2p_{3/2}$ and $2p_{1/2}$ splitting), which resembles the octahedral coordination or pyrite structures (Figure S3c).¹ These observations again confirm that TiB₂ exhibits the strongest polysulfide adsorption ability and TiO_2 is the weakest. Interestingly, it further shows that solvent's structure directly affects how polysulfide adsorb onto the host materials/catalysts thereby affecting the local coordination of sulfur after chemical adsorption.

S L-edge peak assignments for reference samples in Figure S3c¹:

(i) Transition metal sulfides applied octahedral coordination (e.g., TiS₂):

Two sets of doublet features in S L-edge spectra could be assigned to $2p_{3/2}$ and $2p_{1/2}$ to t_{2g} (Ti-3d+S $3p\pi$) and $3e_g$ (Ti-3d+S $3p\pi$), respectively. The energy separation between the doublet peaks is due to the spin-orbit coupling of S 2p electrons and is ~1.2 eV. The energy separation between the 1st and 2nd sets of features is related to the ligand field splitting of t_{2g} and e_g orbitals in octahedral bonding environment.

(ii) Transition metal sulfides applied pyrite structure (FeS₂):

 $S_2^{2^2}$ anion pair is the dominant factor, which is similar to S_8 L-edge feature. Transition metal sulfides applied trigonal prismatic coordination: the first two peaks could be assigned to the excitation from the $2p_{3/2}$ and $2p_{1/2}$ electrons to the E' (d_{xy} ; d_{x2-y2}), and the 3^{rd} peak can be assigned to the excitation from the $2p_{1/2}$ state to the E'' (d_{xz} , d_{yz}). The energy separation between E' and E'' is related to the type of metal element.

Table S2. S L-edge absorption peak positions of XANES of Vulcan carbon and titanium-based compounds (TiB₂, TiC and TiO₂) powders with same total surface area after soaking in Li_2S_8 DOL: DME electrolyte

Peak number	a	b	с	b-a	c-b
	2p _{3/2} →E1	2p _{3/2} →E2	2p _{1/2} →E2	ΔE (E2-E1)	$\Delta E (2p_{3/2}-2p_{1/2})$
TiB_2	163.5	165.6	166.9	1.9	1.3
TiC	163.7	165.5	166.6	1.8	1.1
TiO ₂	N/A	N/A	N/A	N/A	N/A
Vulcan carbon	163.9	165.5	166.6	1.6	1.1

Table S3. S L-edge absorption peak positions of XANES of titanium-based compounds (TiB_2 , TiC and TiO_2) powders with same total surface area after soaking in Li_2S_8 DMSO electrolyte

Peak number	a	b	с	d	b-a	c-b	d-c			
	4-peak separation									
	2p _{3/2} →E1	2p _{1/2} →E2	2p _{3/2} →E2	$2p_{1/2} \rightarrow E2$	ΔE (2p _{3/2} -2p _{1/2})		ΔE (2p _{/3/2} -2p _{1/2})			
TiB ₂	165.7	166.8	167.8	169.0	1.1		1.2			
			3-peak	separation						
	2p _{3/2} →E1	2p _{3/2} →E2	2p _{1/2} →E2		ΔE (E2-E1)	ΔE (2p _{3/2} -2p _{1/2})				
TiC	163.7	165.7	166.8		2	1.1				
			No adso	rption peak						
TiO ₂	N/A	N/A	N/A	N/A	N/A		N/A			



Figure S4. XPS spectra of TiB₂, TiC and TiO₂ pristine powder.



Figure S5. Particle sizes of the nanopowder utilized in this study (TiB₂, TiC and TiO₂). XRD of (a) TiB₂, (b) TiC and (c) anatase TiO₂; bright field TEM and the corresponding particle size distribution histograms of (d) TiB₂, (e) TiC and (f) anatase TiO₂; SEM images and the corresponding particle size distribution histograms of (g) TiB₂, (h) TiC and (i) TiO₂.

Calculation of the crystallite size of TiB₂, TiC and TiO₂ based on Scherrer equation:

$$D = \frac{K\lambda}{\beta cos\theta}$$

where,

D: crystallites size (nm), K: 0.9 (Scherrer constant), λ : 0.15406 nm (wavelength of the X-rage sources), β : FWHM (radians) and θ : peak position (radians).

(hkl)	Peak position (20)	FWHM	Crystallite size (nm)	Average crystallite size (nm)	Statistic average size from TEM	Statistic average size from SEM
TiB ₂						
(001)	27.94	0.20	41.23			
(100)	34.04	0.38	21.97	22.04	24.1	20.1
(101)	44.36	0.44	19.51	22.94	34.1	39.1
(110)	61.35	1.02	9.051			
TiC						
(111)	35.95	0.32	25.78			
(200)	41.78	0.35	24.43			
(220)	60.61	0.41	22.33	22.71	27.7	21.8
(311)	72.57	0.47	21.12			
(222)	76.37	0.51	19.93			
Anatase TiO ₂						
(101)	25.27	0.47	17.24			
(103)	36.95	0.66	12.76			
(004)	37.79	0.62	13.49			
(112)	38.54	0.58	14.49	14.62	25.0	20.7
(200)	48.02	0.47	18.33	14.02	25.0	20.7
(105)	53.93	0.3	12.24			
(211)	55.05	0.54	16.55			
(204)	62.65	0.73	12.65			

Table S4. Average crystallite size of TiB₂, TiC and TiO₂ used in this study from XRD results



Figure S6. Slab models for (a) TiB_2 (001), (b) TiC (111) and (c) $TiO_2(101)$



Figure S7. The most stable structure of Li_2S_8 binding with DMSO molecule. We evaluate the influence of solvent by calculating the binding effect between Li_2S_8 and DMSO molecule, which is stronger than DOL: DME⁴. The most stable structure of Li_2S_8 binding with DMSO molecule is shown in Figure S7. The binding energy between Li_2S_8 and DMSO is -0.96 eV, which is several times lower than that on TiX (X=B, C and O) surfaces (Figure 1). Therefore, it is reasonable to conclude that the solvent would not change the absorption trend observed on various catalysts.

Catalyst	Sulfur loading	Ratio of catalyst/sulfur	SSA of catalyst	Initial capacity	Reference				
•	$(mg_{\rm S} {\rm cm}^{-2})$	•	$[m^2 g^{-1}]$	(C-rate) [mAh g ⁺]					
			Mg-based (XM	g=1.2)					
MgO	2.0	0.67	N/A	1175 (0.05C)	5				
MgB_2	2.0	0.67	102	1270 (0.05C)	5				
Ti-based ($\chi_{Ti}=1.5$)									
TiO.	1.1	1.12	89.23	1083.1 (0.5C)	This work				
110_2	1.0	0.67	N/A	863 (0.5C)	6				
TiN	1.0	0.67	69.7	988 (0.5C)	6				
TiC	3.5	0.64	1611	1100 (0.5C)	7				
ne	1.1	1.9	52.63	1211.1 (0.5C)	This work				
Ti ₂ C	1.0	0.43	67.9	1090 (0.5C)	8				
T;D.	1.1-1.4	2.33	11.6	1232 (0.2C)	9				
11D2	1.1	3.48	28.75	1330.5 (0.5C)	This work				
			V-based (χ_V =	=1.6)					
V_2O_5	2.5	0.25	103	1000 (0.2C)	10				
VO_2	2.5	0.25	103	~1000 (0.2C)	10				
VN	3	0.78	37	1471 (0.2C)	11				
			W-based (xw	=1.7)					
WO_3	2-2.5	1	N/A	1134(0.2C)	12				
WO _{3-x}	2-2.5	1	N/A	1221.1 (0.2C)	12				
WC	1.2-1.5	N/A	2.24	1300 (0.2C)	13				
			Mo-based (XM	_o =1.8)					
MoO_2	1	1.5	70	1100 (0.1C)	14				
MoN _x	1.2-1.5	0.057~0.072	N/A	1298 (0.1C)	15				
Mo_2C	0.8-1.2	0.5	253.6	1298 (0.1C)	16				
			Co-based (XCo	=1.8)					
Co_3O_4	0.6-1	0.33	51.2	1167 (0.2C)	17				
Co ₄ N	1.5-2	0.33	48.4	1441 (0.2C)	18				

Table S5. List of recently reported polar host materials (boride, carbide, nitride and oxide) and their performance parameters.



Figure S8. High frequency intercept of EIS plot of Li-S cells applying TiB_2 , TiC and TiO_2 as the interlayer before cycling, respectively



Figure S9. Schematic illustration of two cell configurations for Li-S batteries used in this study. (a) Normal coin cell with the separator of Celgard (for DOL: DME) or quartz fiber (for DMSO); (b) the polymer-sealed LAGP separated two-compartment cell. Taking advantage of the fact that solid-state electrolyte LAGP ceramic membrane is impermeable to the liquid electrolyte and polysulfide species, two-compartment cell adopted here could help to remove the shuttle effect.



Figure S10. Voltage profiles of the two-compartment cell with LAGP as the separator in (a) DOL: DME at 0.02 C; (b) corresponding differential capacity plots of Li-S batteries in (a); voltage profiles of two compartment cell with LAGP as separator in (c) DMSO at 0.02 C; (d) corresponding differential capacity plots of Li-S batteries in (c).



Figure S11. Galvanostatic tests of TiB₂ functionalized interlayer with and without sulfur electrode. (a) Comparison of TiB₂ functionalized interlayer as the positive electrode and that with sulfur electrode with sulfur loading of 2.2 mg_s (1.1 mg_s cm⁻²) at 0.07 mA (equivalent to 0.02 C); (b) zoom in of the voltage profile in (a) and (c) cycling performance of blank TiB₂ interlayer in DOL: DME electrolyte; (d) comparison of TiB₂ functionalized interlayer as the positive electrode and that with sulfur electrode and that with sulfur electrode with sulfur electrode and that with sulfur electrode with sulfur loading of 2.2 mg_s at 0.07 mA (equivalent to 0.02 C); (e) zoom in of the voltage profile in (d) and (f) cycling performance of blank TiB₂ interlayer in DMSO electrolyte.



Figure S12. Voltage profiles of Li-S batteries under various rates applying DMSO as the electrolytes. (a) Li-S batteries with carbon paper as the interlayer under various rates, no well-defined Li₂S nucleation/growth plateau could be observed when C-rate higher than 0.2 C; (b) comparison of the voltage profiles of Li-S batteries under 0.1 C with TiB₂ or carbon paper interlayer during the first cycle, respectively. 150 mAh g⁻¹ enhance of the discharge capacity was observed with TiB₂ interlayer, which was similar to the results observed in battery applying 0.02 C (Figure 2b).



Figure S13. Rate capability and long cycling performance of Li-S batteries applying TiB₂ coated interlayer. (a) and (b) 1.1 mgs cm⁻² under rates of 0.1 C to 2 C; (c) and (d) 5.6 mgs cm⁻² under rates of 0.05 C to 0.5 C (1C=9.4 mA cm⁻²). (e) Coulombic efficiency (CE) during long-term cycling of Li-S batteries with TiB₂, TiC, TiO₂ and carbon paper as the interlayer at 0.5 C.

TiX	BET area from	Weight for 0.1 m ²	Ratio of TiX/Sulfur	Ratio of	Reference
	Table S1 [m ² g ⁻¹]	[mg]	(loading=1.1 mg	TiX/Sulfur	
			cm^{-2} on $\Phi 16 mm$	(loading=5.6 mg	
			electrode)	cm^{-2} on $\Phi 10$	
				mm electrode)	
TiB ₂	28.75	3.48	1.57	0.79	This work
TiC	19.03	5.25	2.37	1.19	This work
TiO ₂	89.23	1.12	0.51	0.12	This work
Ti ₄ O ₇	290	0.34	0.15		19
VO _x -graphene	103	0.97	0.44		10
Co_3O_4	80.4	1.24	0.56		17
Ti ₂ C	67.9	1.47	0.67		8

Table S6. Calculation of the ratio between catalyst TiX and electrochemically active sulfur



Figure S14. Replications of current-time transients of Li_2S electrodeposition from 0.5 M Li_2S_8 -1M LiTFSI-0.4 M LiNO₃ in DOL: DME under 2.09 V_{Li} (blue) and 2.11 V_{Li} (red), respectively on (a) TiB₂, (b) TiC and (c) TiO₂ decorated carbon paper as the electrode.

Theoretical expressions of the current-time transients

I. Bewick, A., Fleischmann, M., Thirsk, H. (BFT) model ²⁰

2D nucleation with lattice incorporation-controlled growth current transient can be fitted through the BFT model with two forms: (1) instantaneous (2DI) and (2) progressive (2DP).

Instantaneous nucleation (2DI)Progressive nucleation (2DP)
$$J_{2DI}(t) = \frac{2\pi zFMhN_0k_g^2}{\rho}t \exp\left(-\frac{\pi M^2N_0k_g^2}{\rho^2}t^2\right)$$
 $J_{2DP}(t) = \frac{\pi zFMhAN_0k_g^2}{\rho}t^2 \exp\left(-\frac{\pi M^2AN_0k_g^2}{3\rho^2}t^3\right)$ $\frac{j}{j_{max}} = \left(\frac{t}{t_{max}}\right) \left\{ exp\left[\frac{t^2 - t_{max}^2}{2t_{max}^2}\right] \right\}$ (S1) $j_{max} = \left(\frac{t}{t_{max}}\right)^2 \left\{ exp\left[\frac{-2(t^3 - t_{max}^3)}{3t_{max}^3}\right] \right\}$ $t_{max} = \left(\frac{\rho^2}{2\pi M^2N_0k_g^2}\right)^{1/2}$ (S2) $t_{max} = \left(\frac{2\rho^2}{\pi M^2AN_0k_g^2}\right)^{1/3}$ $j_{max} = \frac{(2\pi)^{1/2}zFhN_0^{1/2}k_g}{\rho} \exp\left(-\frac{1}{2}\right)$ (S3) $j_{max} = zFh\left(\frac{4\pi AN_0k_g^2\rho}{M}\right)^{1/3} \exp\left(-\frac{2}{3}\right)$ $j_{max} t_{max} = \frac{zF\rho h}{M} \exp\left(-\frac{1}{2}\right)$ (S4) $j_{max} t_{max} = \frac{2zF\rho h}{M} \exp\left(-\frac{2}{3}\right)$

where $zF[C \text{ mol}^{-1}]$ is the molar charge, $F=96485 \text{ C mol}^{-1}$ is the Faraday constant, $k_g [\text{mol} \text{ cm}^{-2} \text{ s}^{-1}]$ is the nucleus lateral growth-rate constant, h [cm] is the layer thickness, $N_0 [\text{cm}^{-2}]$ and $AN_0 [\text{cm}^{-2} \text{ s}^{-1}]$ are the number density of isolated centers for 2DI and 2DP, respectively, $M [g \text{ mol}^{-1}]$ is the molecular weight, and $\rho [g \text{ cm}^{-3}]$ is the density of the deposited material. Here, $M_{\text{Li2S}}=46 \text{ g mol}^{-1}$, $\rho_{\text{Li2S}}=1.66 \text{ g cm}^{-3}$. The current density $j_{max} [A \text{ cm}^{-2}]$ and the time $t_{max} [s]$, corresponding to the point of the maximum current density, can be evaluated by equating the first derivative to zero. The parameters $N_0k_g^2$ and the layer thickness h [cm] can be determined from the current peak. Both j_{max} and t_{max} are determined by substituting the background current j_0 (final stage) and t_0 (initial stage).







Figure S16. B K-edge spectra of various standard reference samples of $Na_2B_4O_7$ with 4-fold coordinated boron (4c-B), B_2O_3 and H_2BO_3 both with 3-fold coordinated boron (3c-B) and TiB₂ in the FY mode.



Figure S17. Ex-situ B K-edge evolution of the Li-S batteries applying TiB₂-interlayer. (a) Voltage profile of initial cycle of Li-S battery in DMSO. B K-edge spectra evolution under (b) TEY mode and (c) FY mode, respectively.



Figure S18. Experimental (circle) and deconvoluted (lines) of B K-edge spectra from (a) Figure 5b and (b) Figure S17b after subtracting a cubic background of the normalized spectra. Peak A: reduced boron (Boron_{Red}), peak B: oxidized boron (Boron_{Oxi}) take 3-coordination, peak C: oxidized boron and diffuse band of 4-coordinated (C1) and 3-coordinated (C2) boron, respectively²¹⁻²². Boron_{Oxi} and Boron_{Red} evolution during the first cycle in both (c) DOL: DME and (d) DMSO, respectively.

		/ Deals A		Dools D		Peak C				р
No.		rea	ĸА	rear	D	C	l	C	2	\mathbf{D}_{oxi}
	DOC	eV	Area	eV	Area	eV	Area	eV	$\begin{array}{c c} \hline & & & & \\ \hline 2 & & & & \\ \hline Area & & & (\%)^{[a]} \\ \hline \\ \hline 2.08 & 78.87 \\ \hline 3.09 & 94.10 \\ \hline 2.22 & 100 \\ \hline 1.04 & 100 \\ \hline \\ \hline \\ \hline 1.61 & 93.10 \\ \hline 3.28 & 90.56 \end{array}$	(70)
Discharging										
1	21.3%	192.1	0.30	194.17	1.12	198.48	0.49	200.2	2.08	78.87
2	41.4%	192.1	0.17	194.15	2.71	198.83	2.91	201.0	3.09	94.10
3	64.9%	N/A	0	194.22	3.17	198.05	0.59	200.4	2.22	100
4	100%	N/A	0	194.17	1.37	197.92	0.35	201.0	1.04	100
Charging										
5	65%	192.1	0.10	194.18	1.35	198.25	0.32	200.8	1.61	93.10
6	100%	192.1	0.17	194.15	1.63	198.33	0.52	200.8	3.28	90.56
r.1.1.				2. D0/ D						

Table S7. Deconvoluted peak positions and peak areas for B K-edge XANES in DOL: DME shown in Figure S18a

[a] determined by area percentage: 3c-B% = B/(A+B)

Table S8. Deconvoluted peak positions and peak areas for B K-edge XANES in DMSO shown in Figure S18b

No	DoD/	Peak A		Peak B		Peak B				B _{oxi} (%) ^[a]
INO.	DoC				-			B	2	
		eV	Area	eV	Area	eV	Area	eV	Area	
Discharging										
1	14.6%	192.1	0.30	194.17	1.13	198.86	1.11	200.6	1.49	79.02
2	36.7%	192.1	0.41	194.15	1.40	198.95	1.27	200.3	1.76	77.35
3	73.8%	N/A	0	194.22	2.07	197.96	0.38	201.0	0.90	100
4	100%	N/A	0	194.18	1.04	197.99	0.31	199.9	0.44	100
					Chargin	g				
5	29.7%	N/A	0	194.22	1.40	197.89	0.27	200.0	0.66	100
6	62.9%	192.0	0.63	194.19	2.69	198.71	2.05	200.6	4.37	81.02
7	100%	192.1	0.14	194.15	1.34	198.59	0.89	200.4	2.57	90.54

[a] determined by area percentage: 3c-B% = B/(A+B)

Reference

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