Supporting Information for

Quantification of Vehicular versus Uncorrelated Li⁺-Solvent Transport in Highly Concentrated Electrolytes via Solvent-related Onsager Coefficients

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Diffusion coefficients

Table S1: Diffusion coefficients of Li⁺ ions, anions and solvent molecules at different molar ratios $n_{solvent}/n_{salt}$, measured at 30 °C.

system	$n_{solvent}/n_{s}$	D_{Li}^{+}	$D_{A^{-}}$	D _{solvent} /
		$/10^{-12} m^2 s^{-1}$	$/10^{-12} m^2 s^{-1}$	$10^{-12} \text{m}^2 \text{s}^{-1}$
SI /I TESI	2.0/1	3.44 ± 0.28	2.21 ± 0.26	2.93 ± 0.34
SL/L11FSI	3.0/1	10.0 ± 1.18	7.54 ± 0.92	9.61 ± 1.06
CI /I ECI	2.4/1	12.0 ± 0.87	8.44 ± 0.46	8.02 ± 0.53
SL/LIFSI	3.0/1	15.7 ± 1.52	12.8 <u>+</u> 1.29	11.9 ± 1.17
	1.1/1	5.93 ± 0.38	5.79 ± 0.38	7.56 ± 0.50
DMC/LiFSI	1.3/1	10.1 ± 0.67	10.2 ± 0.87	12.9 ± 0.92
	2.0/1	31.5 ± 1.77	35.4 ± 2.17	44.1 ± 2.54

Phase Shift data



ure S1: Representive phase shift data of the electrophoretic NMR measurements on the three DMC-based electrolytes.

Fig



Figure S2: Representative phase shift data of the electrophoretic NMR measurements on the two SL-based electrolytes.



Figure S3: Comparison of the ionic conductivity calculated from ion mobilities (σ_{eNMR}) to that from impedance spectroscopy (σ_{EIS}).

Mobilities

Table S2: Electrophoretic mobilities of Li⁺ ions, anions and solvent molecules at different molar ratios $n_{solvent}/n_{salt}$, measured at 30 °C. The resulting mobility-based anion transference numbers are also listed.

system	n _{solvent} /:	$\mu_{Li}^{\mu_{Li}^{+}}$ /10 ⁻¹¹ m ² (Vs) ⁻¹	$\mu_{A^{-}}$ /10 ⁻¹¹ m ² (Vs) ⁻¹	$\mu_{solvent}$ /10 ⁻¹¹ m ² (Vs) ⁻¹	t_A^{μ}
SL/LiTFSI	2.0/1	9.72 ± 0.95	- 4.07 ± 0.21	2.69 ± 0.47	0.30 ± 0.03
	3.0/1	30.1 ± 2.7	- 17.1 <u>+</u> 2.1	7.81 ± 3.31	0.36 ± 0.05
SL/LiFSI ¹	2.4/1	38.2 ± 4.5	- 19.3 ± 0.3	6.56 ± 1.63	0.33 ± 0.03
	3.0/1	47.0 ± 8.0	- 36.9 ± 5.1	6.10 ± 4.16	0.44 ± 0.08
DMC/LiFSI	1.1/1	9.59 ± 0.91	– 9.82 <u>+</u> 1.35	9.83 ± 1.33	0.51 ± 0.08
	1.3/1	13.6 ± 1.1	- 17.6 ± 1.6	14.6 <u>+</u> 1.5	0.56 ± 0.06
	2.0/1	37.0 ± 7.2	- 61.9 <u>+</u> 11.0	34.6 ± 8.6	0.63 ± 0.14



Figure S4: Exemplary very-low-frequency impedance spectrum of a DMC/LiFSI 1.3/1 electrolyte measured at 30 °C. The red line denotes a fit to the equivalent circuit shown in the inset.



Figure S5: Results of the VLF-EIS measurements for the DMC-based electrolytes. Left: Plot of diffusion resistance R_{diff} versus electrode distance d. Right: Time constant τ versus the squared electrode distance d^2 . The lines denote linear fits.



Figure S6: Results of the VLF-EIS measurements for the SL-based electrolytes. Left: Plot of diffusion resistance R_{diff} versus electrode distance d. Right: Time constant τ versus the squared electrode distance d^2 . The lines denote linear fits.

The linear fits on the left-hand side of Figs. S5 and S6 were used to calculated the Li+ transference number under anion-blocking conditions:

$$t_{Li}^{abc} = \frac{1}{1 + \frac{R_{diff}}{d} \cdot \sigma_{ion} \cdot A}$$
[S1]

Here, A denotes the area of the electrodes.

The linear fits on the right-hand side of Figs. S5 and S6 were used to calculate the salt diffusion coefficient

$$D_{salt} = \frac{d^2}{4 \cdot \tau}$$
[S2]

Concentration cell measurements



Figure S7: Open circuit potentials (OCP) of concentration cells with transference at 30 °C. The electrolytes DMC/LiFSI 1.1/1; 1.3/1 and 2.0/1 were measured versus a 3.365 M DMC/LiFSI reference electrolyte.



Figure S8: Open circuit potentials (OCP) of concentration cells with transference at 30 °C. The electrolytes SL/LiTFSI 2.0/1 and 3.0/1 were measured versus a 2.58 M SL/LiTFSI reference electrolyte

Representative distributions of Onsager coefficients and thermodynamic factors obtained from Monte Carlo-based overdetermination method



Figure S9a: Representative distributions of the Onsager coefficients (left) and the thermodynamic factor (right) for the DMC/LiFSI 1.1/1 system.



Figure S9b: Representative distributions of the Onsager coefficients (left) and the thermodynamic factor (right) for the SL/LiTFSI 3.0/1 system.

Mass densities and partial molar volumes

Table S3: Densities ρ of the studied electrolytes at 30 °C.

system	$n_{solvent}/n_{s}$	ρ / g·cm ⁻³	
CI /I TECI	2.0/1	1.572	
SL/LIITSI	3.0/1	1.502	
	1.1/1	1.569	
DMC/LiFSI	1.3/1 1.528	1.528	
	2.0/1	1.435	

Based on these mass densities at different molar ratios $n_{solvent}/n_{salt}$, the partial molar volume of the solvent, v_0 , and of the salt, v_{salt} , was calculated according to Ref. 5. We assume that the partial molar volume of the Li⁺ ions, v_{Li}^+ , can be approximated by the molar volume of the Li⁺ ions, $V_{M,Li}^+$. Using the ionic radius of a sixfold coordinated Li⁺ ions, $r_{Li}^+ = 76 \text{ pm}^-6$, we calculated the molar volume of the Li⁺ ions as follows:

$$V_{M,Li^{+}} = \frac{4}{3} \cdot \pi \cdot N_A \cdot r_{Li^{+}} = 0.11 \cdot 10^{-5} \frac{m^3}{mol} = v_{Li^{+}}$$
[S3]

Accordingly, the partial molar volume of the anions were calculated as $v_{-} = v_{salt} - v_{Li^+} = v_{salt} - V_{M,Li^+}$.

Table S4: Partial molar volumes of the studied electrolytes at 30 °C.

system	v_0 / 10 ⁻⁵ m ³ /mol	v - / 10 ⁻⁵ m ³ /mol	$V_{M, Li^+} = v_{Li^+ / 10^{-5} \text{ m}^3/\text{mol}}$
SL/LiTFSI	9.55	14.3	0.11
SL/LiFSI1	9.48	9.05	0.11
DMC/LiFSI	8.19	9.12	0.11

Volume conservation



Figure S10: Ratio of the molar volume flux $J_V/J_{V,tot}$ for the DMC/LiFSI and SL/LiTFSI electrolyte systems.

Relations between Onsager coefficients under volume conservation constraint

The Onsager transport equations give the relation between molar fluxes J_i and the thermodynamic forces X_j using the Onsager coefficients $\sigma_{ij:2-4}$

$$J_i = -\sum_{j=1}^n \frac{\sigma_{ij}}{F^2} \cdot X_j$$
 [S4]

Here, n is the total number of mobile species.

In the case of three species (i) cations with index "+", (ii) anions with index "-" and (iii) solvent with index "0", three Onsager equations can be written as:

$$J_{-} = -\frac{\sigma_{+-}}{F^2} \cdot \frac{d\mu_{+}}{dx} - \frac{\sigma_{--}}{F^2} \cdot \frac{d\mu_{-}}{dx} - \frac{\sigma_{-0}}{F^2} \cdot \frac{d\mu_{0}}{dx}$$
[S5a]

$$J_{0} = -\frac{\sigma_{+0}}{F^{2}} \cdot \frac{d\tilde{\mu}_{+}}{dx} - \frac{\sigma_{-0}}{F^{2}} \cdot \frac{d\tilde{\mu}_{-}}{dx} - \frac{\sigma_{00}}{F^{2}} \cdot \frac{d\mu_{0}}{dx}$$
[S5b]

$$J_{+} = -\frac{\sigma_{++}}{F^2} \cdot \frac{d\tilde{\mu}_{+}}{dx} - \frac{\sigma_{+-}}{F^2} \cdot \frac{d\tilde{\mu}_{-}}{dx} - \frac{\sigma_{+0}}{F^2} \cdot \frac{d\mu_0}{dx}$$
[S5c]

If the total volume flux J_v is zero, we have

$$J_v = \sum v_i \cdot J_i = 0$$
 [S6]

with v_i denoting the partial molar volume of species *i*. Since [S6] is valid independent of the acting thermodynamic forces, we can write down the following three relations:

$$v_{+} \cdot \sigma_{+-} + v_{-} \cdot \sigma_{--} + v_{0} \cdot \sigma_{-0} = 0$$
 [S7a]

$$v_{+} \cdot \sigma_{+0} + v_{-} \cdot \sigma_{-0} + v_{0} \cdot \sigma_{00} = 0$$
 [S7b]

$$v_{+} \cdot \sigma_{++} + v_{-} \cdot \sigma_{+-} + v_{0} \cdot \sigma_{+0} = 0$$
 [S7c]

Solving these relations for, σ_{-0} , σ_{00} and σ_{+0} yields:

$$\sigma_{-0} = -\frac{1}{v_0} (v_+ \cdot \sigma_{+-} + v_- \cdot \sigma_{--})$$
 [S8a
]

$$\sigma_{00} = -\frac{1}{v_0} (v_+ \cdot \sigma_{+0} + v_- \cdot \sigma_{-0})$$
 [S8b]

$$\sigma_{+0} = -\frac{1}{v_0} (v_+ \cdot \sigma_{++} + v_- \cdot \sigma_{+-})$$
 [S8c]

Under the assumption that the partial molar volume of the Li⁺ ions, v + , is negligible compared to v - and v_0 , Eqs. [S8a]-[S8c] simplify to:

$$\sigma_{-0} = -\frac{v_{-}}{v_{0}}\sigma_{--}$$
[10]

$$\sigma_{00} = -\frac{v_{-}}{v_{0}} \cdot \sigma_{-0} \approx \left(\frac{v_{-}}{v_{0}}\right)^{2} \cdot \sigma_{--}$$
[11]

$$\sigma_{+0} = \frac{v_{-}}{v_{0}} \cdot \sigma_{+-}$$
[12]

Definition of Li⁺-solvent correlation parameter γ

We start by considering the sum of all displacement vectors of the Li^+ ions:

$$\sum_{i=1}^{N} \Delta \vec{R}_i^{+}(t)$$
[S9]

and the sum over all displacement vectors of the solvent molecules:

$$\sum_{j=1}^{x \cdot N} \Delta \vec{R}_{j}^{\ 0}(t)$$
 [S10]

The summation is done over N cations and $x \cdot N$ solvent molecules, respectively, with $x = n_{solvent}/n_{salt}$ denoting the molar ratio of solvent to salt.

In the case of a *strict vehicular transport mechanisms*, the displacement vector of a Li^+ ion and the displacement vectors of the x solvent molecules bound to this Li^+ ions are identical, implying that:

$$x \cdot \sum_{i=1}^{N} \Delta \vec{R}_i^{+}(t) = \sum_{j=1}^{x \cdot N} \Delta \vec{R}_j^{0}(t)$$
[S11]

$$x \cdot \sum_{i=1}^{N} \Delta \vec{R}_{i}^{+}(t) - \sum_{j=1}^{x+N} \Delta \vec{R}_{j}^{0}(t) = 0$$
 [S12]

Via linear response theory, an Onsager coefficient σ_{ij} can be related to the displacement vectors of the species i and j in equilibrium via:²

$$\sigma_{ij} = \frac{e^2}{6Vk_BT} \lim_{t \to \infty} \frac{d}{dt} \left[\left(\sum_{i=1}^{N_i} \Delta \vec{R}_i(t) \right) \cdot \left(\sum_{j=1}^{N_j} \Delta \vec{R}_j(t) \right) \right]$$
[S13]

Squaring of Eq. [S12] gives:

$$x^{2} \cdot \left[\left(\sum_{i=1}^{N} \Delta \vec{R}_{i}^{+}(t) \right)^{2} \right] + \left[\left(\sum_{j=1}^{x \cdot N} \Delta \vec{R}_{j}^{0}(t) \right)^{2} \right] - 2 \cdot \sum_{i=1}^{N} \Delta \vec{R}_{i}^{+}(t) \sum_{j=1}^{x \cdot N} \Delta \vec{R}_{j}^{0}(t) = 0$$
 [S14]

Inserting the terms of the left-hand side of Eq. [S14] into Eq. [S13] yields:

$$x^2 \cdot \sigma_{++} + \sigma_{00} - 2x \cdot \sigma_{+0} = 0$$
 [S15]

$$x \cdot \sigma_{++} + \frac{1}{x} \sigma_{00} = 2 \cdot \sigma_{+0}$$
 [S16]

Now we define a parameter γ

$$\gamma = \frac{2 \cdot \sigma_{+0}}{x \cdot \sigma_{++} + \frac{1}{x} \sigma_{00}}$$
[13]

which according to Eq. [S16] is unity for a strict vehicular mechanism. Since for uncorrelated movements of Li⁺ ions and solvent molecules, the Onsager coefficient $\sigma + 0$ is zero, the parameter γ is zero as well.

Relationship between the parameters β and γ

Combining the definition of the cation-anion correlation parameter β :

$$\beta = \frac{2 \cdot \sigma_{+-}}{\sigma_{++} + \sigma_{--}}$$
[S17]

and the definition of the cation-solvent correlation parameter γ with Eqs. 11 and 12 yields:

$$\gamma = -\frac{\frac{v_{-}}{v_{0}} \cdot (\sigma_{++} + \sigma_{--})}{x \cdot \sigma_{++} + \sigma_{--} \left(\frac{v_{-}}{v_{0}}\right)^{2} \cdot \frac{1}{x}} \beta$$
[S18]

Since the partial molar volumes v_{-} and v_{0} , the Onsager coefficients σ_{++} and σ_{--} and the molar ratio x are all positive, the parameters γ and β exhibit opposite signs.

Measured parameters and target values

Table S5: Compilation of all experimental quantities measured for the SL/LiTFSI system as well as of all transport quantities derived from the experimental results.

SL/LiTFSI	Unit	2.0/1	3.0/1
t_{Li}^{μ}		0.70 (± 0.09)	0.64 (± 0.07)
σ_{ion}	S/m	0.042 (± 0.003)	0.098 (± 0.006)
t_{Li}^{abc}		0.50 (± 0.08)	0.32 (± 0.03)
D _{salt}	$10^{-11} \text{ m}^{2/\text{s}}$	3.0 (± 1.0)	3.3 (± 0.5)
$\frac{d\Delta\varphi}{d\ln\left(c_{salt}\right)}$	V	0.150 (± 0.04)	0.09 (± 0.08)
σ_{++}/σ_{ion}		$0.55~(\pm 0.08)$	0.41 (± 0.04)
$\sigma_{}/\sigma_{ion}$		0.32 (± 0.20)	0.32 (± 0.10)
σ_{+-}/σ_{ion}		-0.12 (± 0.09)	-0.15 (± 0.04)
thermodyn. factor		5.6 (± 1.2)	4.8 (± 0.7)
β		-0.28 (± 0.22)	-0.41 (± 0.12)
σ^{self}_{+}	10-2 S/m	3.7 (± 0.3)	8.5 (± 0.3)
σ^{self}_{-}	10-2 S/m	2.4 (± 0.3)	$6.4 (\pm 0.8)$
$\sigma^{distinct}_{++}/\sigma^{self}_{+}$		-0.38 (± 0.15)	-0.53 (± 0.16)
$\sigma^{distinct} / \sigma^{self}$		-0.44 (± 0.38)	-0.51 (± 0.22)
σ_{+0}	10-2 S/m	$0.8~(\pm 0.6)$	2.2 (± 0.6)
σ_{-0}	10-2 S/m	-2.0 (± 1.3)	-4.7 (± 1.5)
σ_{00}	10 ⁻² S/m	3.0 (± 1.1)	7.1 (± 1.3)
σ_0^{self}	10-2 S/m	6.4 (± 0.7)	24.6 (± 2.7)
$\sigma^{distinct}_{00}/\sigma^{self}_{0}$		-0.53 (± 0.23)	-0.71 (± 0.16)
1/		$0.25 (\pm 0.19)$	0.31 (+ 0.09)

 γ 0.25 (± 0.19)
 0.31 (± 0.09)

 Table S6: Compilation of all experimental quantities measured for the SL/LiFSI system as well as of all transport quantities derived from the experimental results.¹

SL/LiFSI	Unit	2.4/1	3.0/1
$t^{\mu}_{Li^+}$		0.66 (± 0.10)	0.56 (± 0.11)
σ_{ion}	S/m	0.156 (± 0.013)	0.194 (± 0.004)
t^{abc}_{Li+}		0.23 (± 0.02)	0.29 (± 0.02)
D _{salt}	10 ⁻¹¹ m ² /s	$1.2 (\pm 0.2)$	3.2 (± 0.9)
$\frac{d\Delta\varphi}{d{\ln\left(c_{salt}\right)}}$	V	0.091 (± 0.015)	0.073 (± 0.017)
σ_{++}/σ_{ion}		0.36 (± 0.06)	0.39 (± 0.02)
$\sigma_{}/\sigma_{ion}$		$0.26~(\pm 0.08)$	0.28 (± 0.02)
σ_{+-}/σ_{ion}		-0.19 (± 0.02)	-0.16 (± 0.02)
thermodyn. factor		4.3 (± 0.7)	3.7 (± 0.8)
β		-0.61 (± 0.11)	$-0.48 (\pm 0.06)$
σ^{self}_{+}	10-2 S/m	13.9 (± 1.0)	15.4 (± 1.5)

σ^{self}_{-}	10-2 S/m	9.8 (± 0.5)	12.5 (± 1.3)
$\sigma^{distinct}_{++}/\sigma^{self}_{+}$		-0.60 (± 0.15)	-0.51 (± 0.11)
$\sigma^{distinct} / \sigma^{self}$		-0.59 (± 0.17)	-0.57 (± 0.12)
σ_{+0}	10 ⁻² S/m	$2.8 (\pm 0.4)$	3.0 (± 0.4)
σ_{-0}	10-2 S/m	-3.9 (± 1.3)	-5.2 (± 0.4)
σ_{00}	10-2 S/m	3.7 (± 1.6)	$5.0 (\pm 0.8)$
σ^{self}_{0}	10 ⁻² S/m	22.3 (± 1.5)	34.9 (± 3.4)
$\sigma^{distinct}_{00}/\sigma^{self}_{0}$		-0.83 (± 0.16)	-0.86 (± 0.13)
γ		$0.38 (\pm 0.06)$	$0.24 (\pm 0.03)$

Table S7: Compilation of all experimental quantities measured for the DMC/LiFSI system as well as of all transport quantities derived from the experimental results.

DMC/LiFSI	Unit	1.1/1	1.3/1	2.0/1
t_{Li}^{μ}		0.49 (± 0.06)	$0.44~(\pm 0.04)$	0.37 (± 0.09)
σ_{ion}	S/m	0.098 (± 0.03)	0.151 (± 0.006)	0.363 (± 0.015)
t^{abc}_{Li} +		0.37 (± 0.08)	0.32 (± 0.08)	0.28 (± 0.023)
D _{salt}	10 ⁻¹¹ m ² /s	0.6 (± 0.2)	$2.1 (\pm 0.8)$	5.3 (± 0.9)
$\frac{d\Delta\varphi}{d{\ln\left(c_{salt}\right)}}$	V	0.14 (± 0.04)	0.15 (± 0.07)	0.17 (± 0.03)
σ_{++}/σ_{ion}		$0.38 (\pm 0.06)$	$0.37 (\pm 0.06)$	$0.30 (\pm 0.03)$
$\sigma_{}/\sigma_{ion}$		$0.37 (\pm 0.09)$	0.51 (± 0.09)	0.62 (± 0.11)
σ_{+-}/σ_{ion}		-0.13 (± 0.04)	$-0.06 (\pm 0.06)$	$-0.04 (\pm 0.05)$
thermodyn. factor		4.7 (± 0.9)	5.2 (± 1.0)	5.4 (± 0.8)
β		-0.35 (± 0.12)	-0.14 (± 0.14)	-0.09 (± 0.11)
σ^{self}_{+}	10 ⁻² S/m	$12.0 (\pm 0.8)$	18.8 (± 1.3)	45.4 (± 2.6)
σ^{self}_{-}	10-2 S/m	11.7 (± 0.8)	19.0 (± 1.6)	51.0 (± 3.1)
$\sigma^{distinct}_{++}/\sigma^{self}_{+}$		-0.69 (± 0.10)	-0.70 (0.11)	$-0.76 (\pm 0.09)$
$\sigma^{distinct}_{}/\sigma^{self}_{}$		-0.69 (± 0.12)	-0.59 (± 0.13)	-0.56 (± 0.12)
σ_{+0}	10 ⁻² S/m	$1.4 (\pm 0.4)$	$1.0 (\pm 1.0)$	1.6 (± 2.0)
σ_{-0}	10 ⁻² S/m	$-4.0 (\pm 1.0)$	-8.6 (± 1.6)	-25.1 (± 4.7)
σ_{00}	10-2 S/m	4.5 (± 1.2)	9.6 (± 1.9)	27.9 (± 5.6)
σ_0^{self}	10 ⁻² S/m	16.8 (± 1.1)	31.2 (± 2.2)	127.1 (± 7.3)
$\sigma^{distinct}_{00}/\sigma^{self}_{0}$		-0.73 (± 0.11)	-0.69 (± 0.12)	-0.78 (± 0.10)
γ		0.35 (± 0.12)	0.14 (± 0.14)	0.09 (± 0.11)

G4/LiFSI System

Table S8: Summary of data for the G4/LiFSI system reported before⁷ and the new calculated parameters $\sigma + 0$, $\sigma - 0$, σ_{00} and γ .

G4/LiFSI	Unit	1.0/1	1.5/1	2.0/1
σ_{ion}	S/m	0.158	0.195	0.245
ρ	g/cm ³	1.32	1.24	1.09
σ_{++}/σ_{ion}		$0.30 (\pm 0.07)$	0.34 (± 0.06)	$0.40 (\pm 0.04)$
$\sigma_{}/\sigma_{ion}$		0.52 (± 0.16)	0.84 (± 0.41)	1.14 (± 0.32)
σ_{+-}/σ_{ion}		-0.38 (± 0.01)	-0.39 (± 0.04)	$-0.45 (\pm 0.03)$
β		-0.93	-0.66	-0.58
σ_{+0}	10-2 S/m	1.6	1.6	1.9
σ_{-0}	10 ⁻² S/m	-2.2	-3.5	-4.8
σ_{00}	10 ⁻² S/m	0.9	1.5	2.0
γ		0.82	0.54	0.42

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