

Supporting Information

Lithium Salt/Amide-Based Deep Eutectic Electrolytes for Lithium Ion Battery: Electrochemical, Thermal and Computational Study

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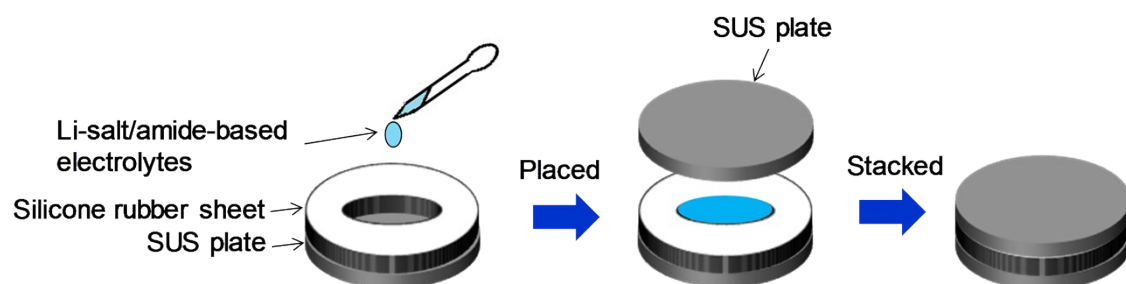


Figure S1. Schematic illustrations of preparation of a cell for ionic conductivity measurement.

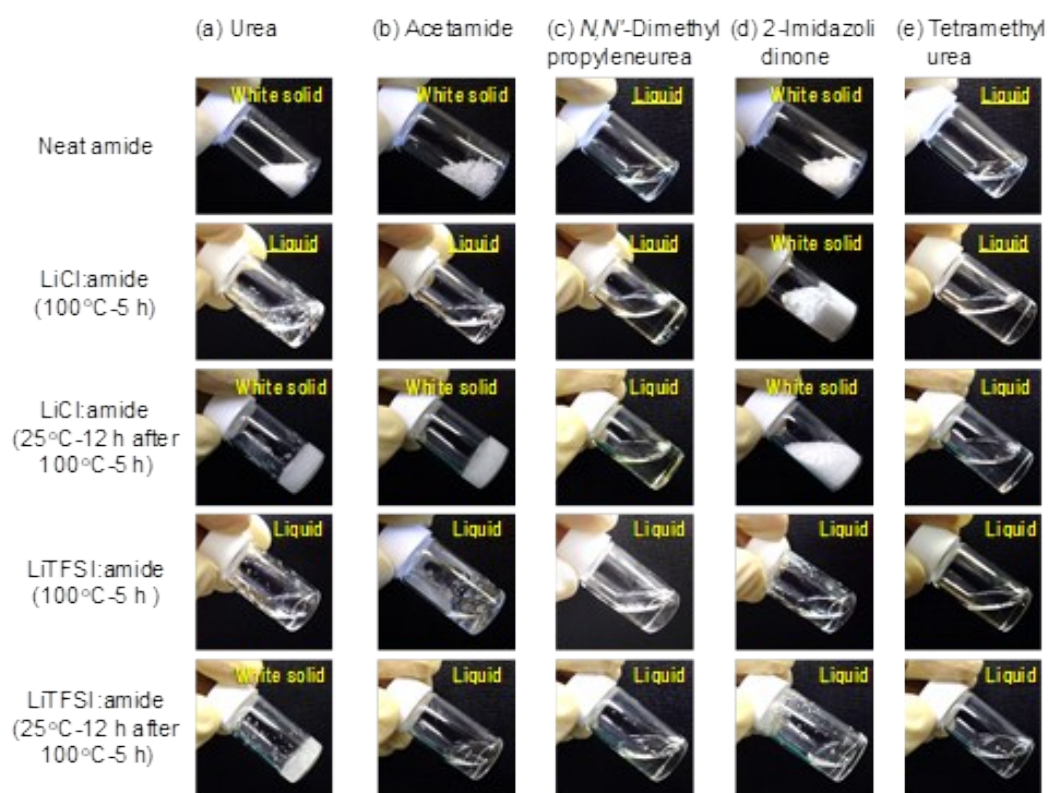


Figure S2. The appearances of the neat amides (before heating), LiCl/amide-based electrolytes (i.e. LiCl:amide = 1:5 mol%) and LiTFSI/amide-based electrolytes (i.e. LiTFSI:amide = 1:5 mol%) comprising (a) urea, (b) acetamide, (c) *N,N'*-dimethylpropyleneurea, (d) 2-imidazolidinone and (e) tetramethylurea, respectively. The conditioning temperature is as described in this figure.

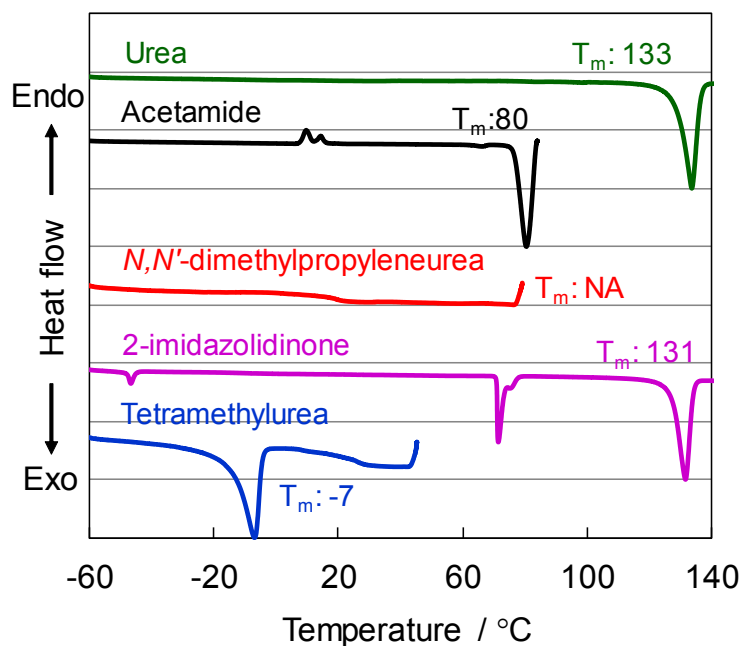


Figure S3. DSC curves of the neat amides.

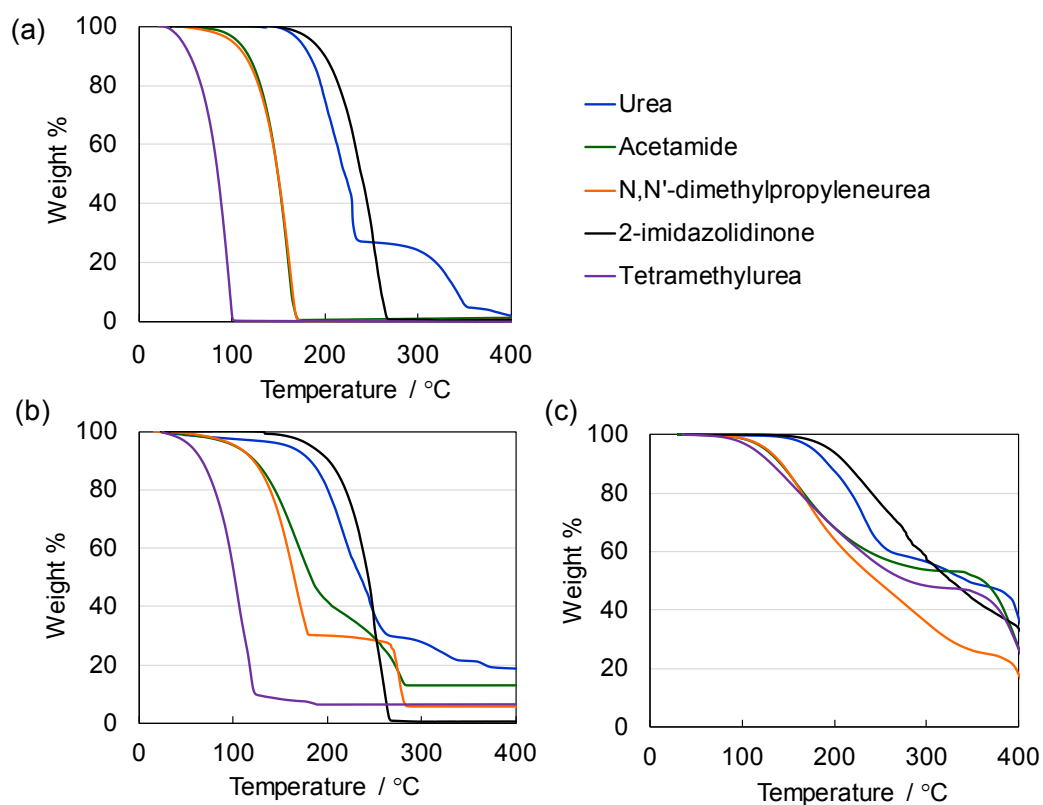


Figure S4. TGA curves of (a) neat amides and (b) LiCl/amide based electrolytes (LiCl:amide = 1:5 mol%), (c) LiTFSI/amide based electrolytes (LiTFSI:amide = 1:5 mol%).

Table S1. Binding energies (BE) of amides and lithium salts.

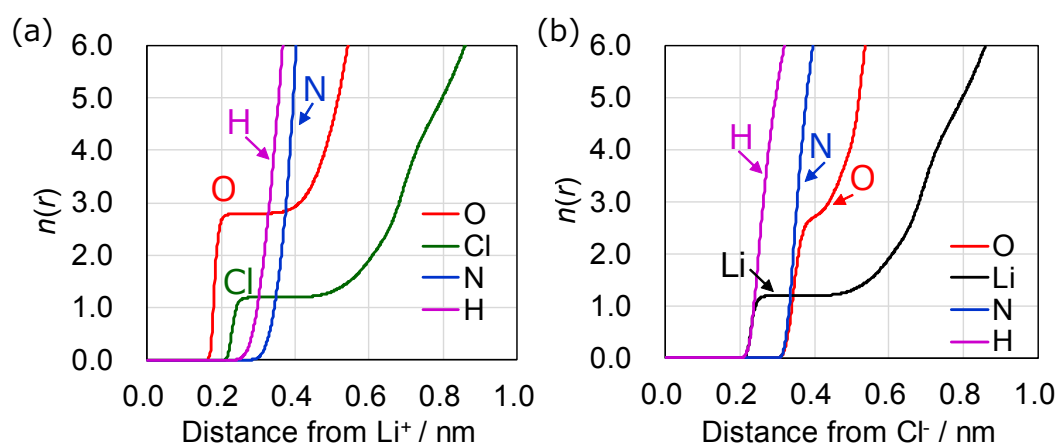
complex	BE _{sol+Li} [kcal mol ⁻¹]	BE _{sol+anion} [kcal mol ⁻¹]
Urea + Li ⁺	-60.7	-
Urea + Cl ⁻	-	-26.6
Urea + TFSI ⁻	-	-16.7
Tetramethylurea + Li ⁺	-65.3	-
Tetramethylurea + Cl ⁻	-	-11.2
Tetramethylurea + TFSI ⁻	-	-8.6

Table S2. The coordination distance of each atoms from Cl⁻ in LiCl/amide-based electrolytes estimated from RDF.

Sample	O in amide	N in amide	H in amide	Li ⁺
LiCl:urea = 1:5 mol%	0.34	0.34	0.24	0.23
LiCl:tetramethylurea = 1:5 mol%	0.35	0.35	0.26	0.23

Table S3. The coordination distance of each atoms from N⁻ in TFSI⁻ in LiTFSI/amide-based electrolytes estimated from RDF.

Sample	O in amide	N in amide	H in amide	Li ⁺
LiTFSI:urea = 1:5 mol%	0.51	0.32	0.23	0.20
LiTFSI:tetramethylurea = 1:5 mol%	0.33	0.50	0.30-0.62	0.20

**Figure S5.** The coordination number $n(r)$ of each atoms in LiCl:urea = 1:5 mol% electrolyte around (a) Li⁺ and (b) Cl⁻.

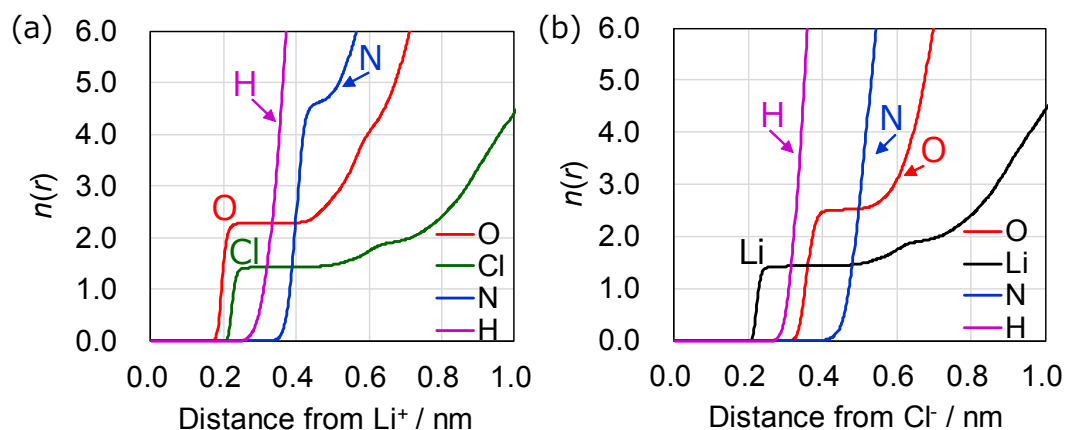


Figure S6. The coordination number $n(r)$ of each atoms in LiCl:tetramethylurea = 1:5 mol% electrolyte around (a) Li^+ and (b) Cl^- .

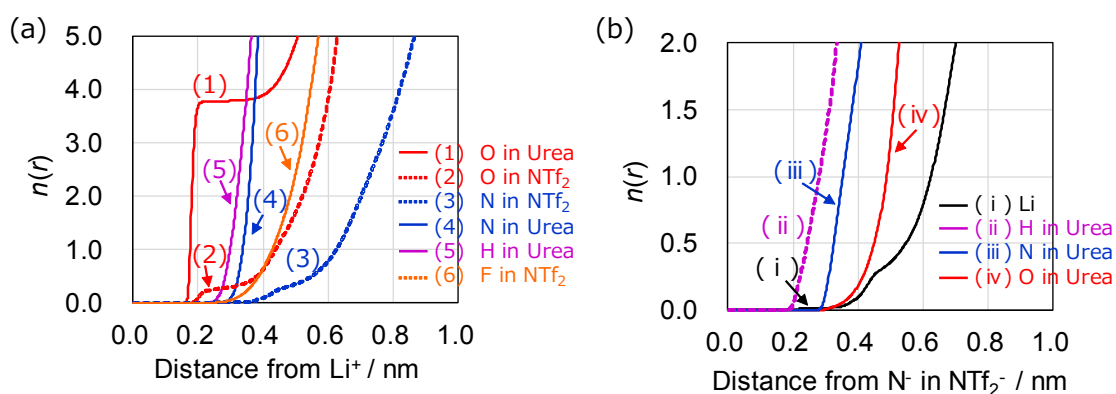


Figure S7. The coordination number $n(r)$ of each atoms in LiTFSI:urea = 1:5 mol% electrolyte around (a) Li^+ and (b) N^- in TFSI $^-$.

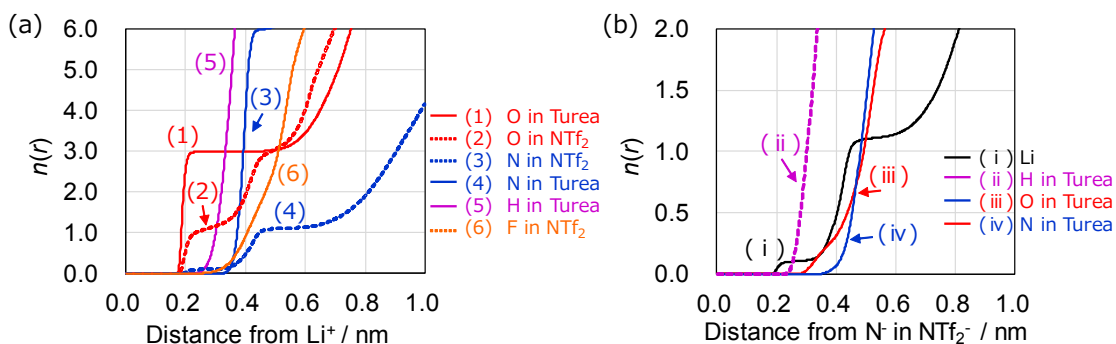


Figure S8. The coordination number $n(r)$ of each atoms in LiTFSI:tetramethylurea = 1:5 mol% electrolyte around (a) Li^+ and (b) N^- in TFSI $^-$.

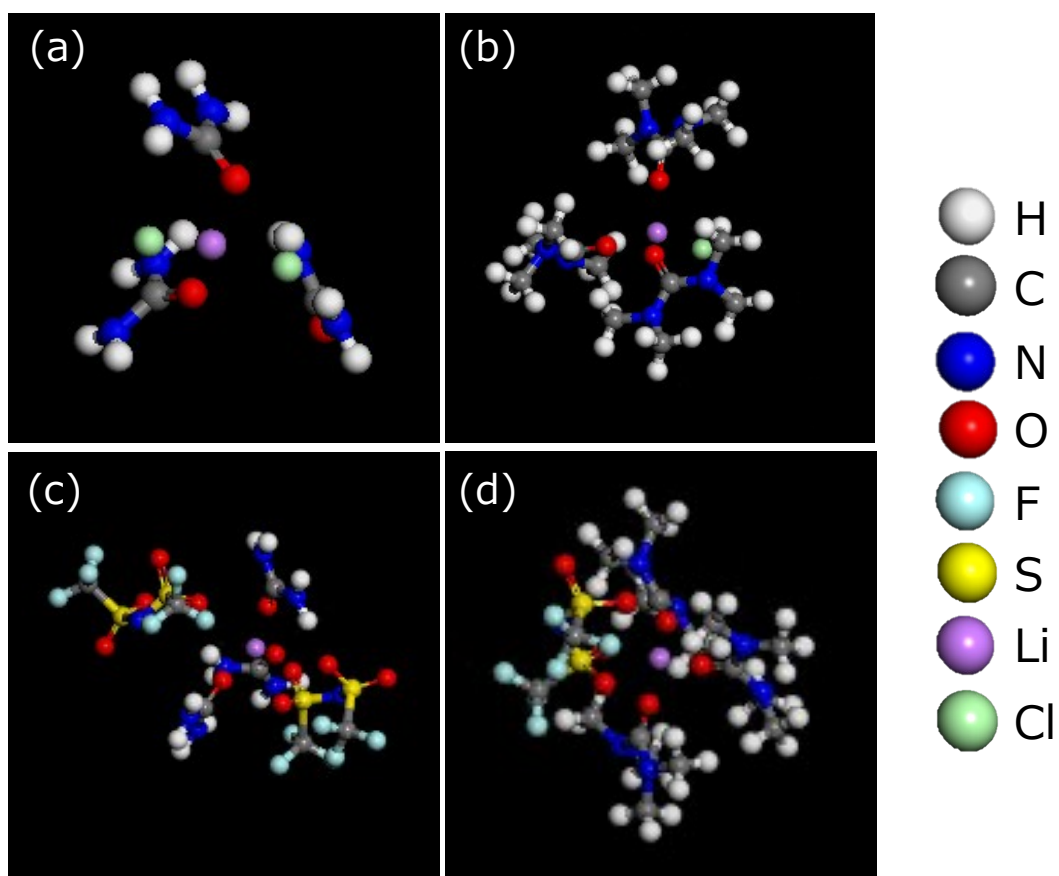


Figure S9. Typical coordination diagrams of molecules existing 3 Å from Li⁺ center of (a) LiCl:Urea = 1:5 mol%, (b) LiCl:Tetramethylurea = 1:5 mol%, (c) LiTFSI:Urea = 1:5 mol%, and (d) LiTFSI:Tetramethylurea = 1:5 mol%.