

Supporting Information

Key features of organic electrolyte molecules in lithium ion battery

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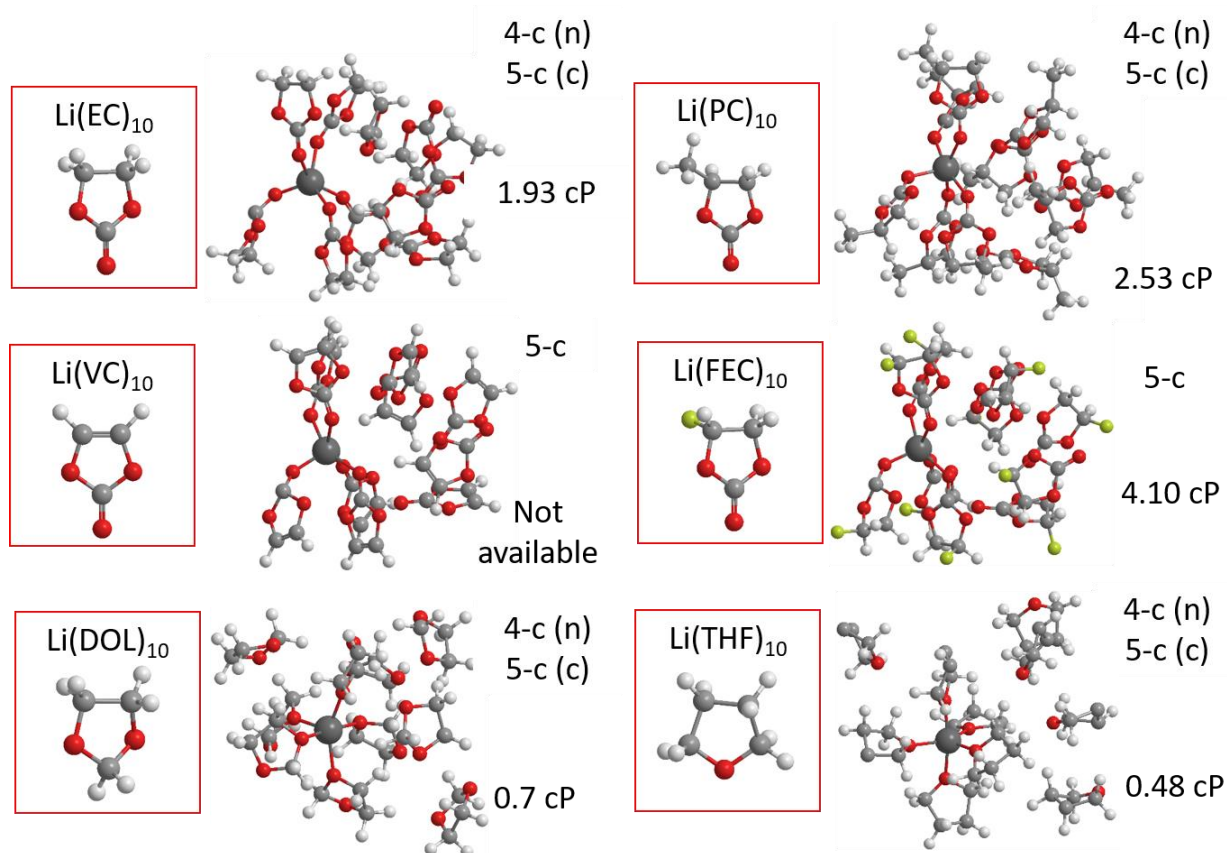
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Fig. S1. The images of the optimum geometries of lithium complexes with 14 types of ten organic electrolyte molecules. The coordination numbers of the optimum complexes, four-coordination (4-c) and five-coordination (5-c), are shown for neutrals (n) and cations (c). The viscosity is also shown in centipoise (cP).



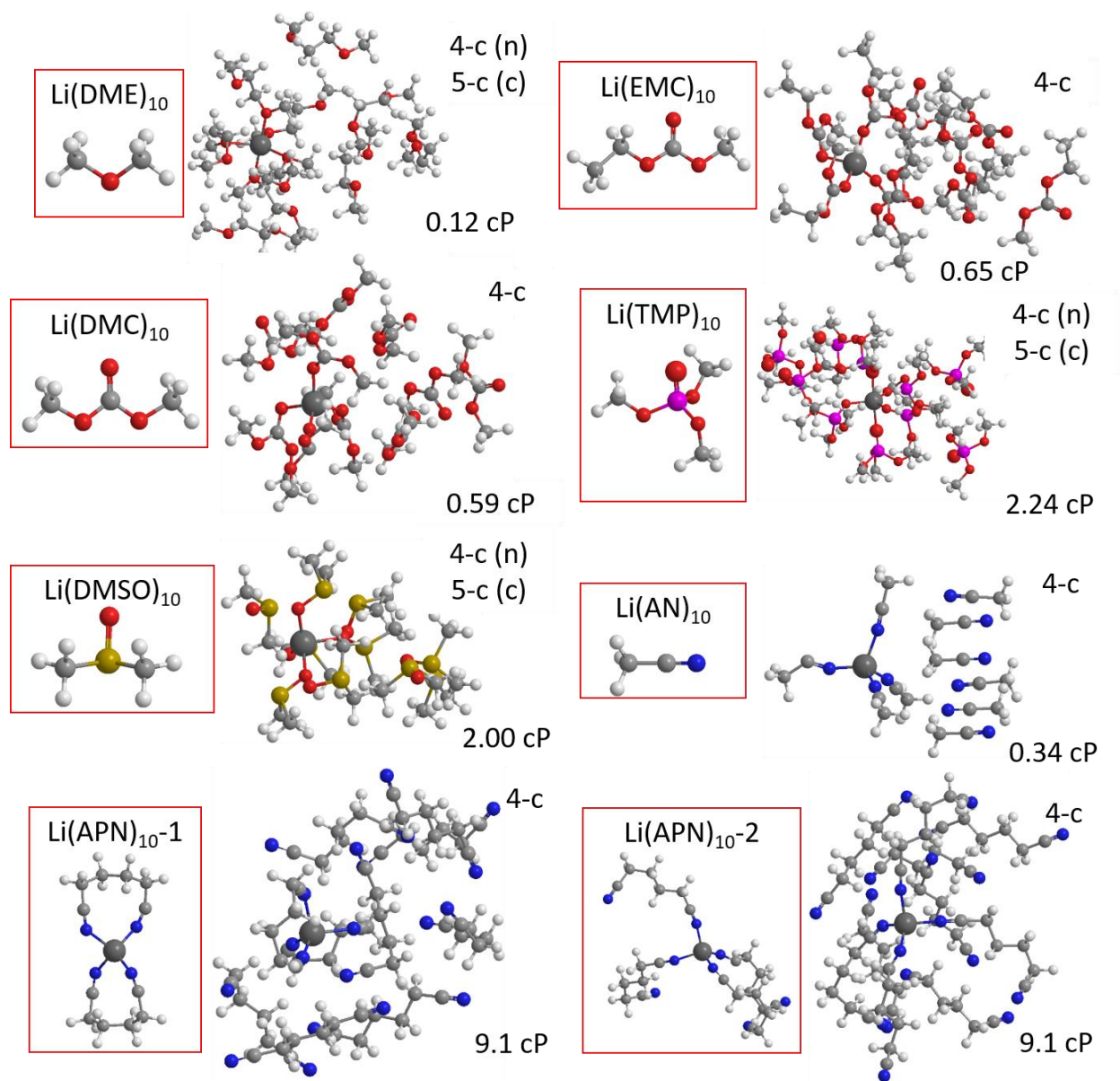
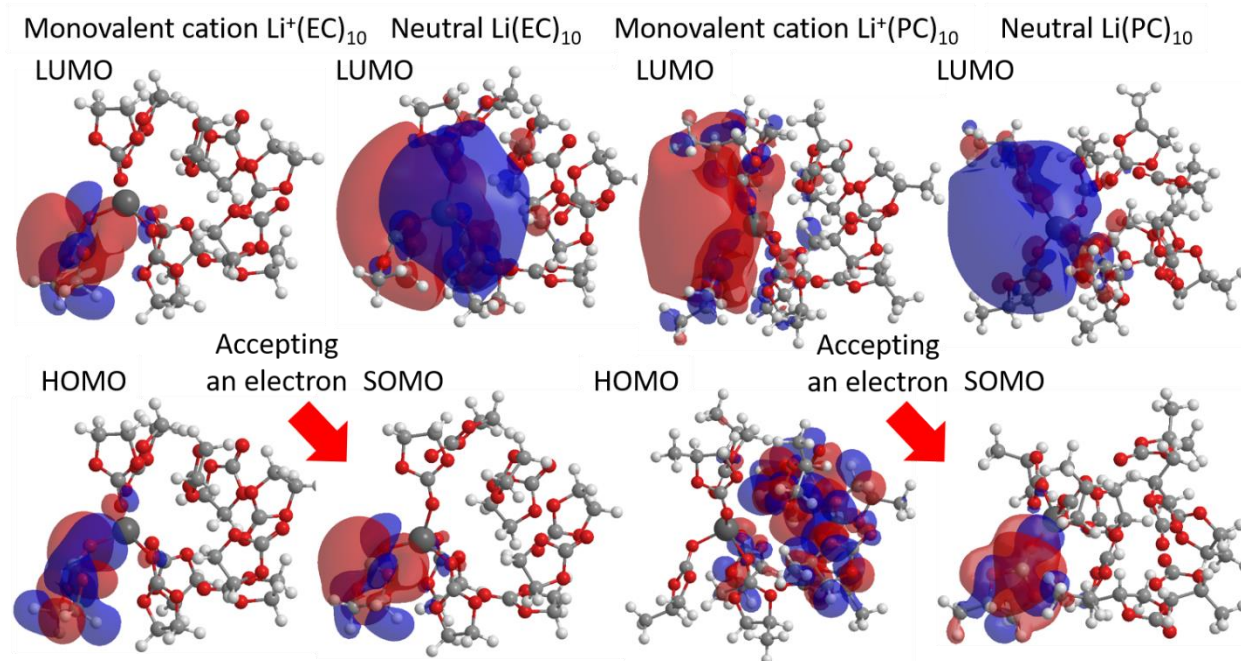
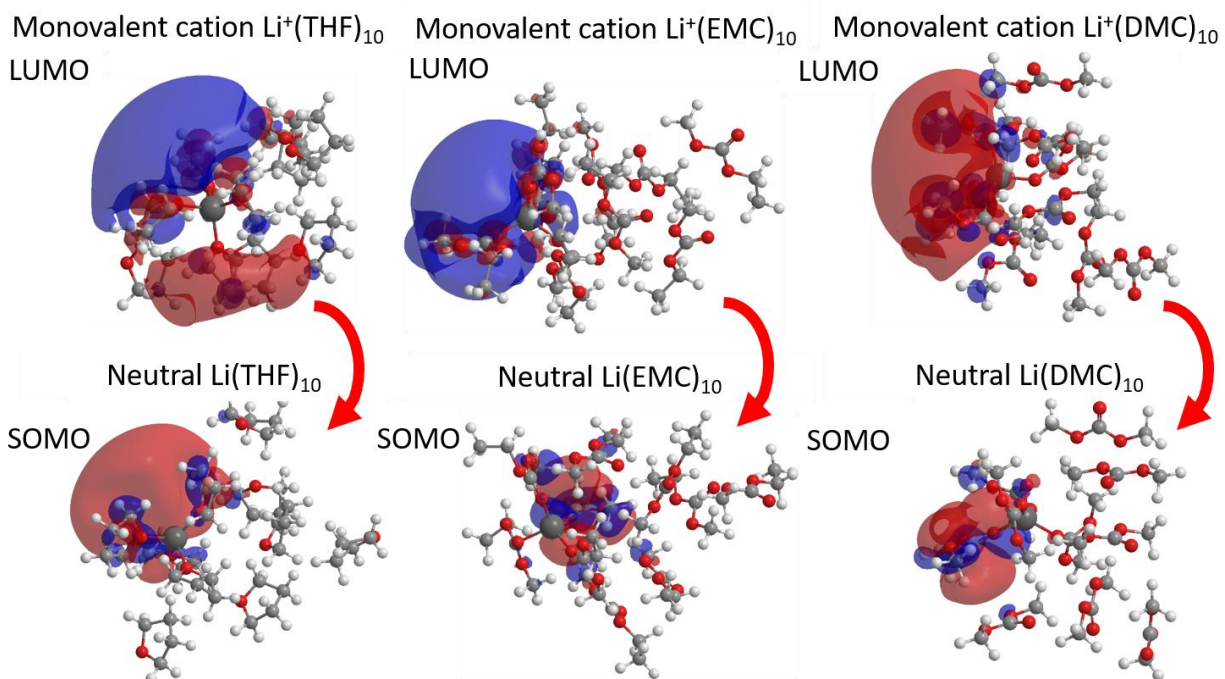
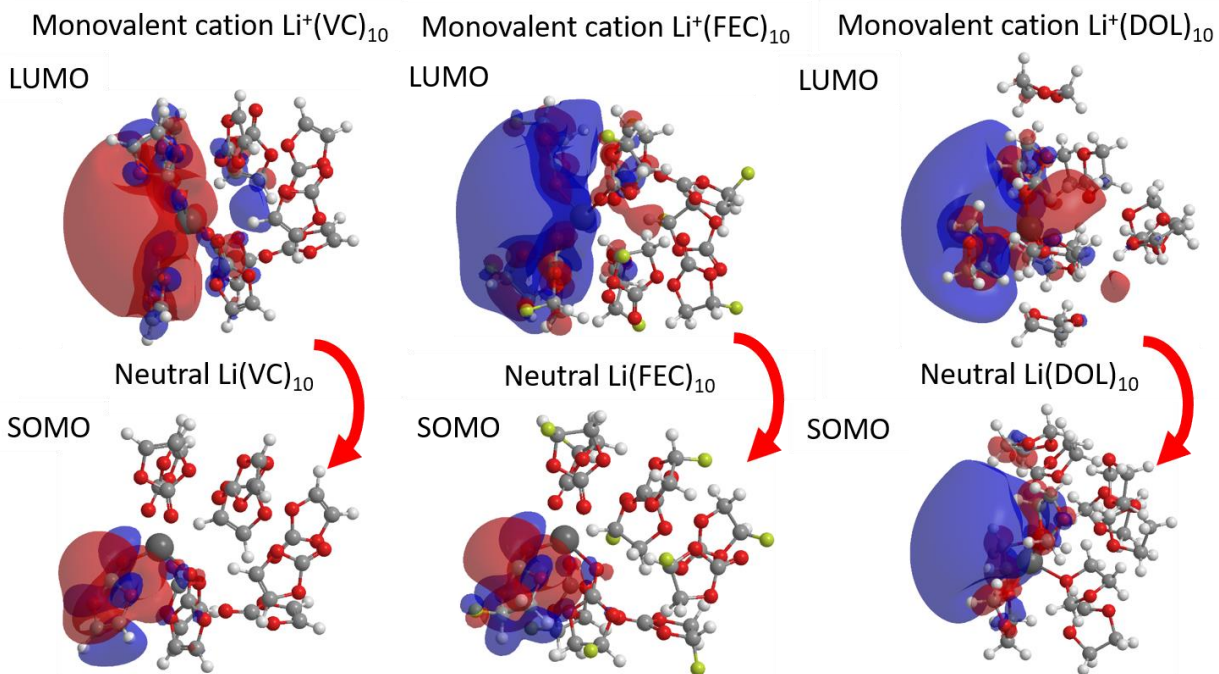
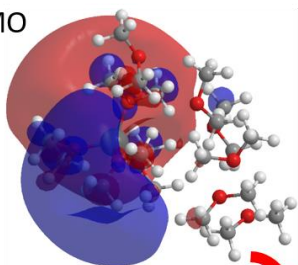


Fig. S2. The molecular orbital images of the LUMOs of the monovalent cations and the SOMOs of the neutrals for lithium complexes with 14 types of ten organic electrolyte molecules. For EC and PC, the HOMOs of the monovalent cations and the LUMOs of the neutrals are also shown.



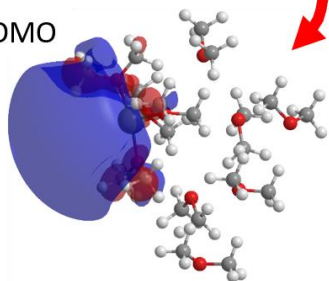


Monovalent cation $\text{Li}^+(\text{DME})_{10}$
LUMO

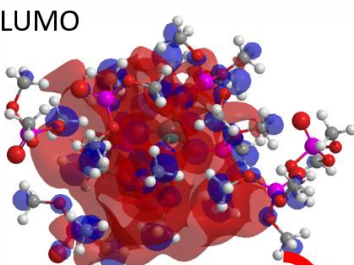


Neutral $\text{Li}(\text{DME})_{10}$

SOMO

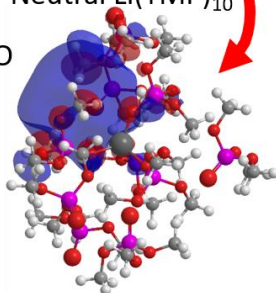


Monovalent cation $\text{Li}^+(\text{TMP})_{10}$
LUMO

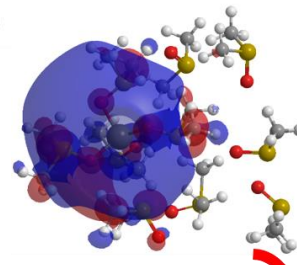


Neutral $\text{Li}(\text{TMP})_{10}$

SOMO

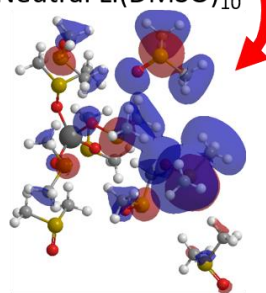


Monovalent cation $\text{Li}^+(\text{DMSO})_{10}$
LUMO

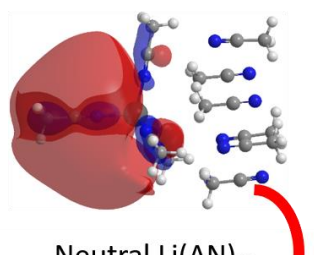


Neutral $\text{Li}(\text{DMSO})_{10}$

SOMO

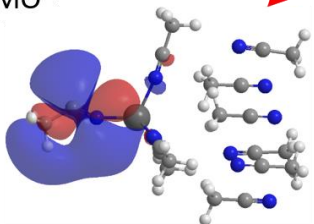


Monovalent cation $\text{Li}^+(\text{AN})_{10}$
LUMO

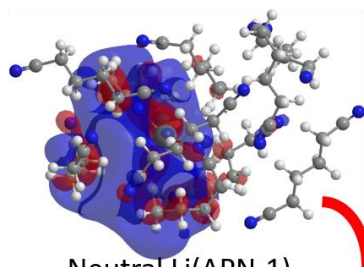


Neutral $\text{Li}(\text{AN})_{10}$

SOMO

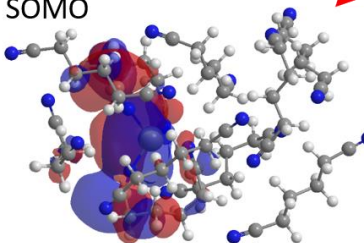


Monovalent cation $\text{Li}^+(\text{APN-1})_{10}$
LUMO

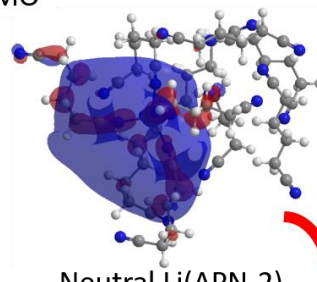


Neutral $\text{Li}(\text{APN-1})_{10}$

SOMO



Monovalent cation $\text{Li}^+(\text{APN-2})_{10}$
LUMO



Neutral $\text{Li}(\text{APN-2})_{10}$

SOMO

