ADVANCED ENERGY MATERIALS

Supporting Information

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Electrostatic Potential as Solvent Descriptor to Enable Rational Electrolyte Design for Lithium Batteries

Yanzhou Wu, Qiao Hu, Hongmei Liang, Aiping Wang, Hong Xu, Li Wang and Xiangming He**

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1. Supporting figures.

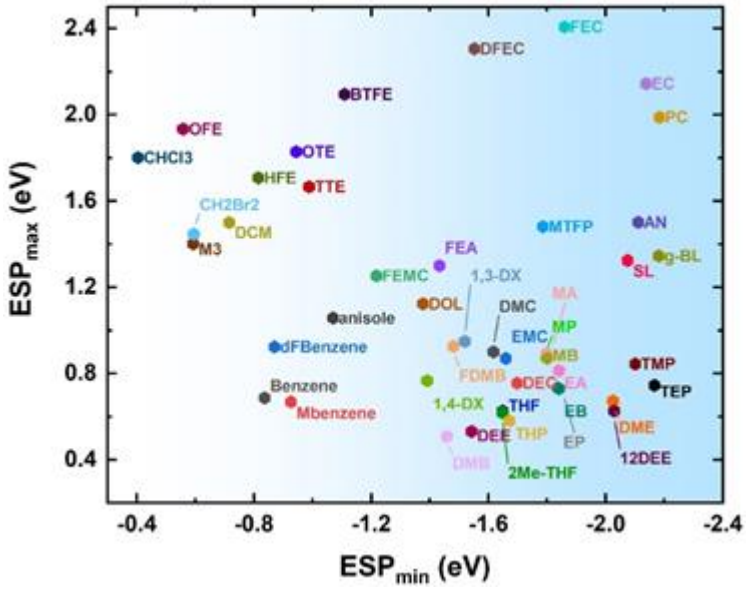

Figure S1. Density functional theory-calculated electrostatic potential (ESP) of various solvents in acetone.

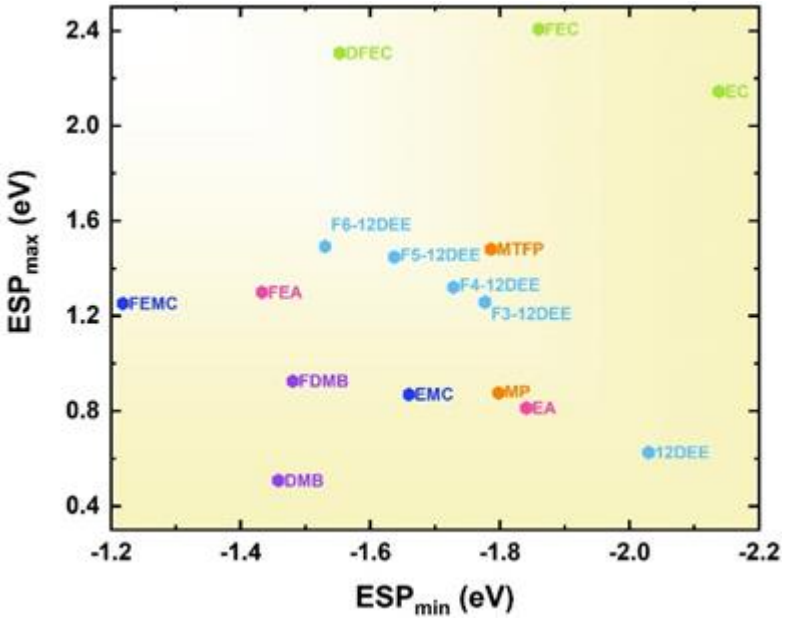

Figure S2. ESP of fluorinated solvents in acetone.

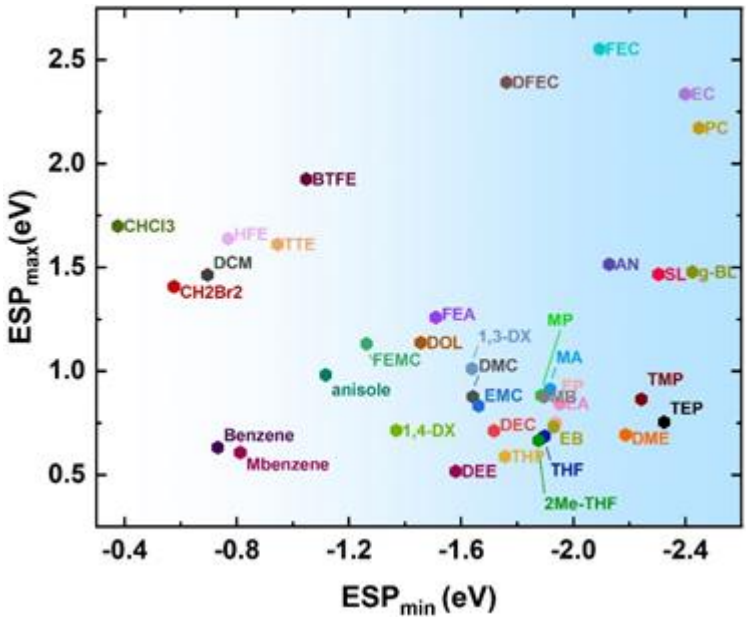

Figure S3. Density functional theory-calculated electrostatic potential (ESP) of various solvents in solution conditions.

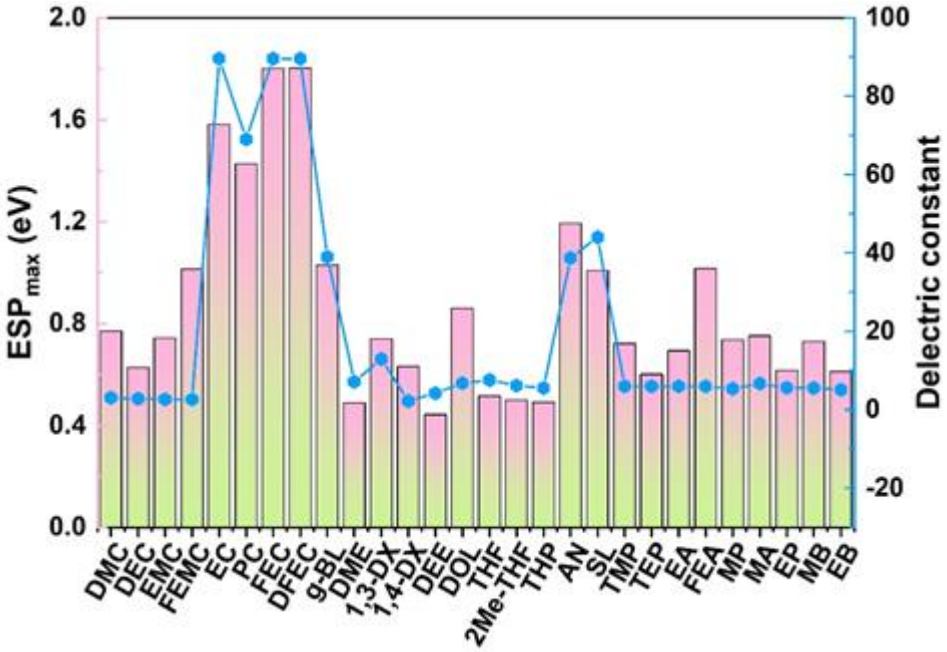

Figure S4. ESP_{max} (left layer) and the dielectric constant (right layer) of solvating solvents in vacuum conditions.

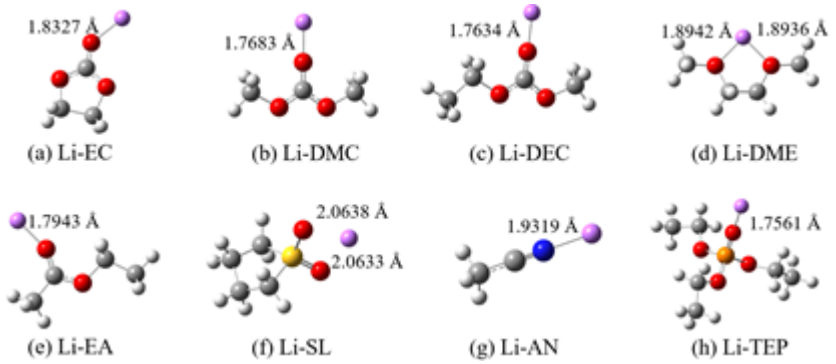

Figure S5. Optimized chemical structures of various Li^+-solvent complexes in acetone conditions. Li, O, H, S, N, and P atoms are shown are purple, red, gray, yellow, blue, and orange, respectively.

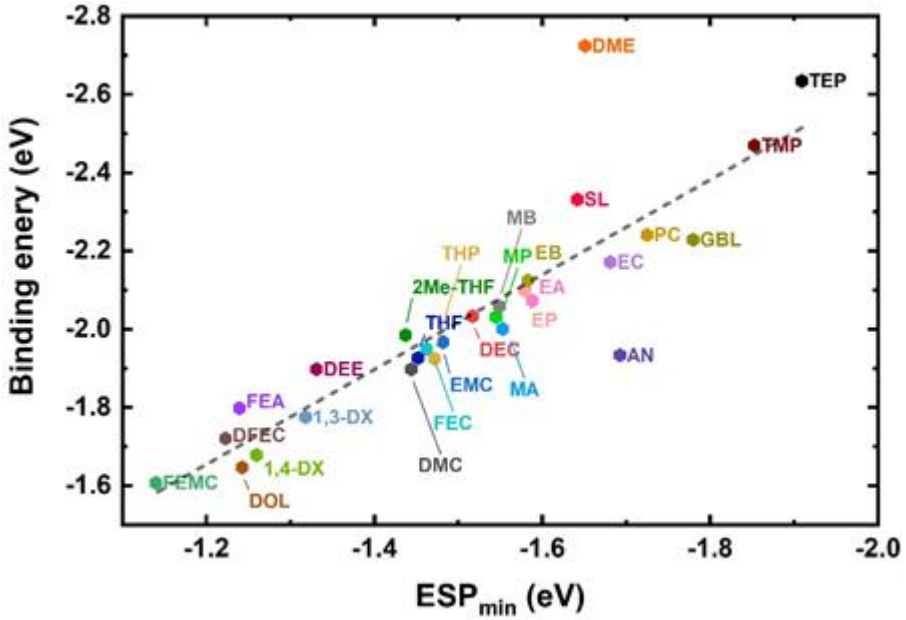

Figure S6. Comparison of two scales for solvents: binding energy and ESP_{min} in gas.

Table S1. Parameters for SMD in this work.

Solvent	Dielectric constant	Solvent	Dielectric constant
DMC	3.09	TMP	6
DEC	2.82	TEP	6
EMC	2.64	EA	6.02
FEMC	2.64	FEA	6.02
EC	89.6	MP	5.4
PC	69	MA	6.7
FEC	89.6	EP	5.65
DFEC	89.6	MB	5.6
g-BL	39	EB	5.1
DME	7.2	HFE	6.4
1,3-DX	13	TTE	6.2
1,4-DX	2.2	BTFE	4.3
DEE	4.27	DCM	5.9
DOL	6.79	CHCl3	5.1
THF	7.58	CH2Br2	7.8

2Me-THF	6.24	Benzene	2.3
THP	5.61	Mbenzene	2.4
AN	38.8	Anisole	4.3
SL	44	Acetone	20.7

Table S2. The full name and abbreviation of organic solvents mentioned in this work.

Solvent	Abbreviation	Solvent	Abbreviation
Dimethyl carbonate	DMC	Methyl acetate	MA
Diethyl carbonate	DEC	Ethyl Propanoate	EP
Ethyl methyl carbonate	EMC	Methyl butyrate	MB
Trifluoroethyl methyl carbonate	FEMC	Ethyl butyrate	EB
Ethylene carbonate	EC	1,4-dimethoxylbutane	DMB
Propylene carbonate	PC	Fluorinated 1,4-dimethoxylbutane	FDMB
Fluoroethylene carbonate	FEC	1,2-diethoxyethane	12DEE
Difluoroethylene carbonate	DFEC	Fluorinated-1,2-diethoxyethane derivant1[a]	F3-12DEE
γ-butyrolactone	GBL	Fluorinated-1,2-diethoxyethane-derivant2[a]	F4-12DEE
1,2-dimethoxyethane	DME	Fluorinated-1,2-diethoxyethane-derivant3[a]	F5-12DEE
1,3-dioxane	1,3-DX	Fluorinated-1,2-diethoxyethane-derivant4[a]	F6-12DEE
1,4-dioxane	1,4-DX	Anisole	Anisole
Diethyl ether	DEE	1,1,2,2-tetrafluoroethyl-2,2,2-trifluoroethyl ether	HFE
1,3-dioxolane	DOL	1,1,2,2-tetrafluoroethyl 2,2,3,3-tetrafluoropropyl ether	TTE
Tetrahydrofuran	THF	Bis(2,2,2trifluoroethyl) ether	BTFE

2-Methyltetrahydrofuran	2Me-THF	1H,1H-octaffuoropentyl-1,1,2,2-tetraffuoroethyl ether	OFE
Tetrahydropyran	THP	1H,1H,5H-octafluoropentyl 1,1,2,2-tetrafluoroethyl ether	OTE
Acetonitrile	AN	(tetrafluoro1-(2,2,2-trifluoroethoxy) ethane	M3
Sulfolane	SL	Dichloromethane	DCM
Trimethyl phosphate	TMP	Trichloromethane	$CHCl_3$
Triethyl phosphate	TEP	Dibromomethane	CH_2Br_2
Ethyl acetate	EA	Benzene	Benzene
Ethyl fluoroacetate	FEA	Methylbenzene	Mbenzene
Methyl propionate	MP	1,2-difluorobenzene	dFbenzene
Methyl 3,3,3-trifluoropionate	MTFP		

[a]: The solvents given here are found from previous publication.[1]

Reference

[1] Z. Yu, P. E. Rudnicki, Z. Zhang, Z. Huang, H. Celik, S. T. Oyakhire, Y. Chen, X. Kong, S. C. Kim, X. Xiao, H. Wang, Y. Zheng, G. A. Kamat, M. S. Kim, S. F. Bent, J. Qin, Y. Cui, Z. Bao, *Nature Energy* **2022,** *7*, 94.