



Low Li⁺ binding affinity: An important characteristic for additives to form solid electrolyte interphases in Li-ion batteries

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ABSTRACT

Calculations are made of the lowest unoccupied molecular orbital (LUMO), chemical hardness (η), dipole moment (μ), and binding energy with a Li⁺ ion for 32 organic molecules that are electrolyte additives for solid electrolyte interphase (SEI) formation in lithium-ion batteries (LIBs). The results confirm that both the LUMO and η values are critical indicators of suitable SEI formation. The μ values of the additives are generally smaller than those of widely used solvents in LIBs. It is found that a low Li-ion binding affinity may be an important characteristic for SEI-forming additives. Li⁺ binding affinity is proposed as a factor in the computational screening process used to obtain promising additives.

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1. Introduction

For lithium-ion batteries (LIBs), the electrolyte typically consists of one or more lithium salts dissolved in an aprotic solvent, often with at least one additive. Additives are included in electrolyte formulation to perform specific functions. A common function is to enhance electrode stability by facilitating the formation of the solid electrolyte interphase (SEI) layer. In LIBs using a graphite anode, various simple organic molecules act as anode SEI additives. They are selected to control the chemistry at the anode|electrolyte interface. The SEI plays a vital role in the reactions of LIBs, and is also a key material for cycle life, lifetime, power capability, and even safety. The initial step towards anode SEI formation is electron transfer to the SEI-forming species that results in a single- or multi-step decomposition reaction to produce the passivating SEI layer at the graphite|electrolyte interface [1–3].

A higher reduction potential than the solvent would therefore be an important requirement for electrolyte additives selected to protect the electrolyte solvent from decomposition. The lowest unoccupied molecular orbital (LUMO) energy or electron affinity (EA) values have been used as a key screening factor for the develop-

ment of SEI-forming additives in LIBs [4]. Computational screening is the cornerstone of *in silico* (via computer simulation) material discovery, as it allows researchers to identify promising structures efficiently. Computational evaluation is faster and much less expensive than experimental trial-and-error testing when effective screening factors are known [5].

Recently, Halls and Tasaki [4] proposed an SEI-forming additive using a high-throughput virtual screening technique; they calculated the LUMO, EA, chemical hardness (η), and dipole moment (μ). It was reported that a small η value and a low LUMO energy would be favourable characteristics of an SEI-forming additive, because a small η implies high reactivity.

This study examines the dipole moment (μ) and binding energy with a Li⁺ ion (BE(Li⁺)) of SEI-forming additives. Halls and Tasaki reported [4] that an effective anodic SEI-forming additive may possess a significant μ , as a larger value of μ leads to stronger non-bonding interaction with Li⁺ to form stable lithium adducts as SEI film components, although this may not always be a requirement. The LUMO, η , μ , and BE(Li⁺) for 32 SEI-forming additives [6–36] (see Fig. 1) have been calculated and it is confirmed that the LUMO and η values are critical indicators of suitable SEI formation.

2. Computational details

Density functional theory (DFT) has become a popular method for calculating molecular properties for a vast array of organic

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molecules used in LIBs [37–40]. The ground-state structures of the molecules have been fully optimized within C1 symmetry by means of DFT methods. The Kohn–Sham equation was calculated with the B3PW91 functional and 6-311G(d,p) basis sets of triple- ζ quality. The functional includes a three-parameter adiabatic connection exchange term [41]: a linear combination of the exact Hartree–Fock exchange, Slater exchange [42], and B88 gradient-corrected exchange [43].

This study employs the conductor-variant polarized continuum model (CPCM) [44], which places the solute in a molecular-shaped cavity imbedded in a continuum dielectric medium. In the CPCM, the variation of the free energy when going from vacuum to solution is composed of the work required to build a cavity in the solvent (cavitation energy) together with the electrostatic (solute–solvent interaction and solute polarization) and non-electrostatic work (dispersion and repulsion energy). A dielectric constant of 31.9 was adopted as a weighted average value between the dielectric constants of ethylene carbonate (EC: 89.2) and ethyl methyl carbonate (EMC: 2.9), because an EC:EMC = 1:2 solution is widely used as the solvent in LIBs [1,45]. All of the DFT

and CPCM calculations were performed with the program package Gaussian 03 [46].

3. Results and discussion

The LUMO, η , μ , $BE(Li^+)_{gas}$ and $BE(Li^+)_{sol}$ values of 32 additives are listed in Table 1, with the EC and propylene carbonate (PC) results shown for comparison. The addition of SEI-forming additives to PC-based solutions greatly suppresses solvent decomposition and graphitic exfoliation in LIBs [47]. The present calculations confirm that both the LUMO and η values are critical indicators of suitable SEI formation. The LUMO energies of all the additives are lower than that of the EC (or PC) value, and there are only two exceptions (4.54 eV for additive **4** and 4.56 eV for **5**) for the lower chemical hardness with respect to EC (4.53 eV). The data support the Halls–Tasaki [4] approach of using the LUMO and η values to search effectively for SEI-forming candidates.

It is worth noting that the μ values (0.37–6.20 D) of additives are, in general, smaller than the EC μ value of 5.34 D (or PC value of 5.52 D), which is in good agreement with the experimental value

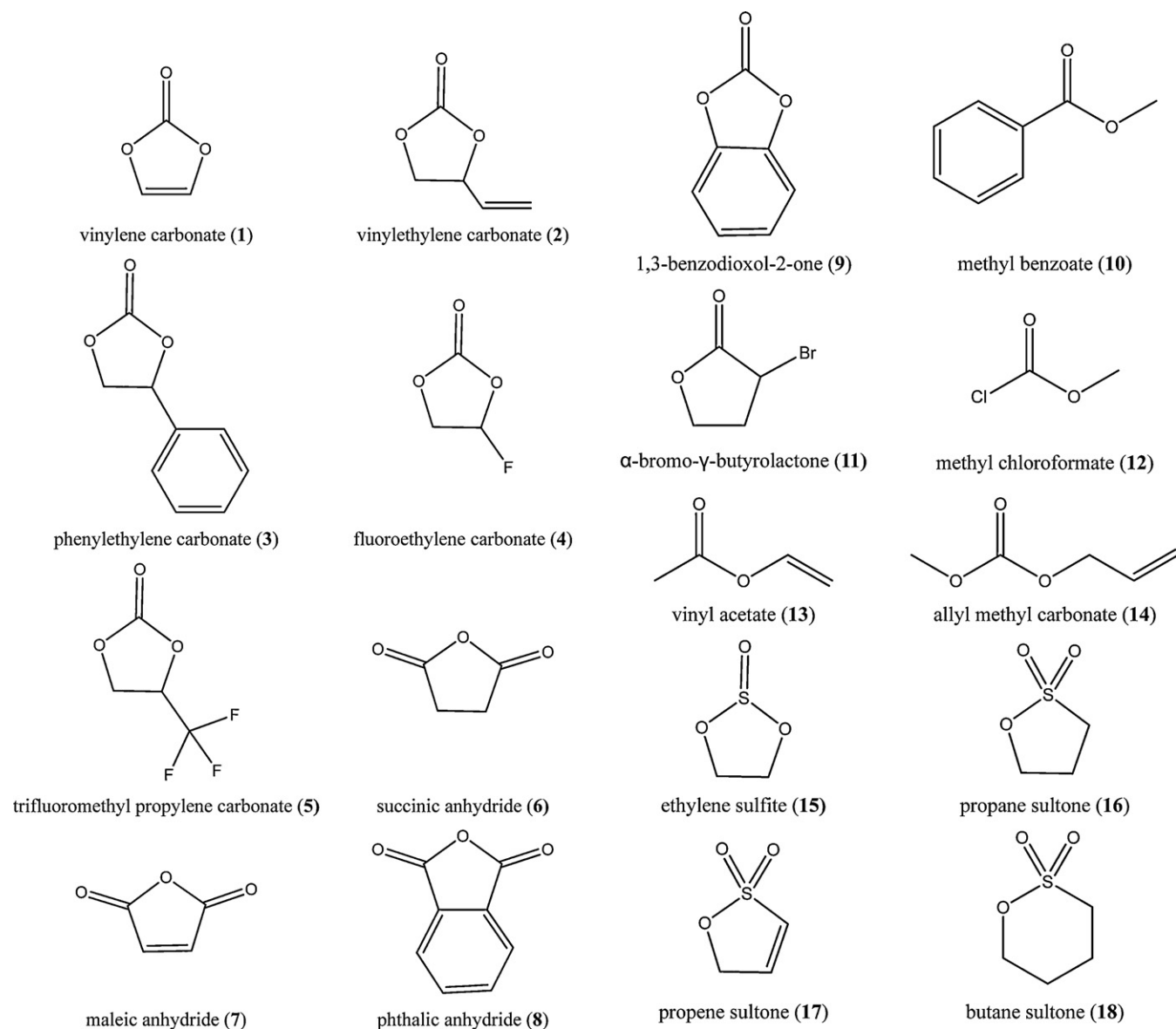


Fig. 1. Thirty-two organic additives for SEI formation in LIBs.

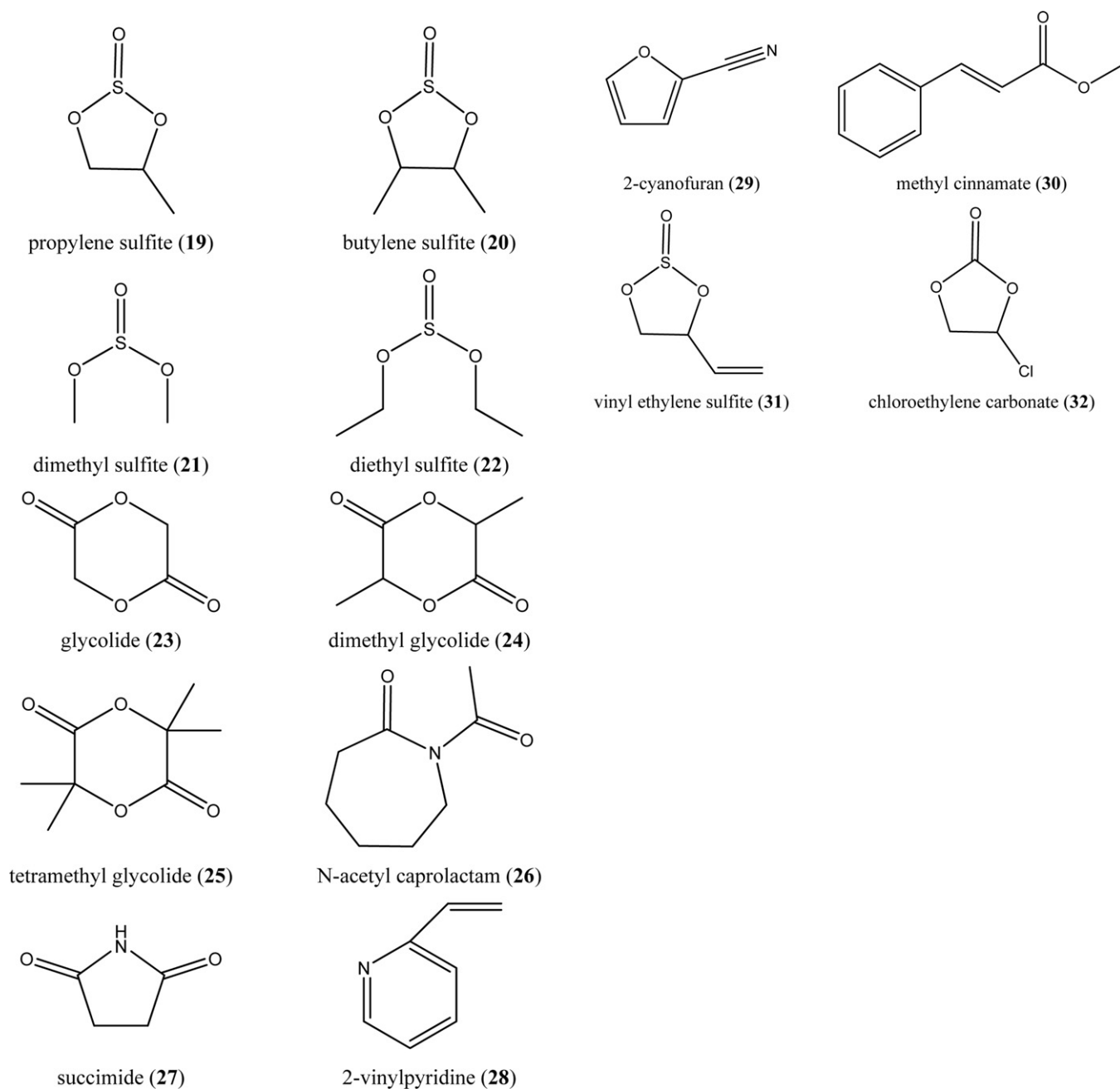


Fig. 1. (Continued).

of 5.35 D [48]. Exceptionally, the three SO_3 -containing additives (16–18) have larger μ values (>6.0 D). It is reasonable to assume that the dipole moment is related, to some degree, to the binding energy between an additive and a Li^+ ion because its main attractive interaction is an ion–dipole interaction. The $\text{BE}(\text{Li}^+)_{\text{gas}}$ values (1.70–2.36 eV) of the additives are generally smaller, i.e., more weakly bonding, than the EC and PC values of 2.24 and 2.32 eV, respectively. It is noted that a large dipole moment does not guarantee a large $\text{BE}(\text{Li}^+)_{\text{gas}}$. For instance, the μ values of SO_3 -containing additives (16–18) are large (>6.0 D), and bond more weakly with Li^+ than EC. That the μ values are not directly proportional to $\text{BE}(\text{Li}^+)_{\text{gas}}$ can be partly explained by the fact that a Li^+ ion may, or may not, interact with the molecular dipole directly (e.g., 1 and 7), depending on structural characteristics, as shown in Fig. 2. It is worth noting that the weaker interactions between additives and Li^+ are

more clearly indicated by the $\text{BE}(\text{Li}^+)_{\text{sol}}$ values, which are the Li^+ binding affinities in solution. The $\text{BE}(\text{Li}^+)_{\text{sol}}$ values (0.01–0.28 eV) of the additives are smaller than the EC and PC values of 0.29 and 0.31 eV, respectively. Such discrepancies between the relative orders of $\text{BE}(\text{Li}^+)_{\text{gas}}$ and $\text{BE}(\text{Li}^+)_{\text{sol}}$ can be rationalized by considering the relationship between molecular volume and solvation energy. A previous study [49] reported that it is often difficult to stabilize additives with large molecular volume by solvent solvation. For instance, the volumes of additive 3 (185.5 \AA^3), 22 (160.2 \AA^3) and 30 (202.7 \AA^3) are much larger than that of EC (92.8 \AA^3), leading to the following orders of values: $30 > 3 > 22 > \text{EC}$ and $\text{EC} > 30 > 22 > 3$ for $\text{BE}(\text{Li}^+)_{\text{gas}}$ and $\text{BE}(\text{Li}^+)_{\text{sol}}$, respectively.

A more realistic model has been tested, $\text{Li}^+(\text{EC})_2(\text{additive})$ [50] for 1 and 7. The $\text{BE}(\text{Li}^+)_{\text{sol}}$ results are presented in Table 2 and are in good agreement with the results of the simple Li^+ -additive model,

Table 1
Lowest unoccupied molecular orbital (LUMO), chemical hardness (η), dipole moment (μ), Li^+ binding energy ($\text{BE}(\text{Li}^+)$), and molecular volume (\AA^3) of 32 SEI-forming additives. Results for EC and PC included for comparison.

Material	LUMO (eV)	η (eV)	μ (debye)	$\text{BE}(\text{Li}^+)$ (eV)		Volume (\AA^3)	Ref.
				Gas	Solvent		
(1) Vinylene carbonate	-0.26	3.47	4.59	2.06	0.24	87.74	[6–8]
(2) Vinylethylene carbonate	-0.84	3.60	5.55	2.31	0.28	129.58	[9,10]
(3) Phenylethylene carbonate	-0.89	3.23	5.23	2.29	0.25	185.54	[11]
(4) Fluoroethylene carbonate	0.37	4.54	4.74	2.03	0.22	100.52	[12–14]
(5) Trifluoromethyl propylene carbonate	0.36	4.56	4.60	2.04	0.22	135.96	[15,16]
(6) Succinic anhydride	-1.02	3.49	4.46	1.91	0.18	106.44	[17]
(7) Maleic anhydride	-3.41	2.49	4.10	1.76	0.14	101.84	[18]
(8) Phthalic anhydride	-2.86	2.66	5.76	2.00	0.15	158.38	[19]
(9) 1,3-Benzodioxol-2-one	-1.09	2.99	4.49	2.07	0.17	143.23	[20]
(10) Methyl benzoate	-1.48	2.93	1.85	2.15	0.22	166.56	[20]
(11) α -Bromo- γ -butyrolactone	-1.10	3.33	4.84	2.26	0.17	130.35	[21]
(12) Methyl chloroformate	-0.39	4.07	2.91	1.70	0.13	96.36	[21]
(13) Vinyl acetate	-0.53	3.28	1.69	1.96	0.20	111.04	[22]
(14) Allyl methyl carbonate	-0.24	3.70	0.37	2.01	0.20	143.08	[22]
(15) Ethylene sulfite	-0.77	3.61	3.63	2.07	0.23	104.27	[23]
(16) Propane sultone	0.52	4.41	6.04	2.13	0.04	121.10	[24]
(17) Propene sultone	-1.55	3.28	6.20	2.12	0.03	114.87	[25]
(18) Butane sultone	0.44	4.40	6.01	2.18	0.01	140.01	[26]
(19) Propylene sulfite	-0.71	3.59	3.89	2.14	0.23	125.01	[27]
(20) Butylene sulfite	-0.64	3.55	3.97	2.16	0.20	145.84	[28]
(21) Dimethyl sulfite	0.14	4.05	2.35	2.07	0.10	118.56	[29,30]
(22) Diethyl sulfite	-0.20	3.65	1.86	2.25	0.26	160.26	[29,30]
(23) Glycolide	-0.83	3.66	2.43	1.84	0.22	116.98	[31]
(24) Dimethyl glycolide	-0.72	3.59	1.93	1.98	0.21	158.55	[32]
(25) Tetramethyl glycolide	-0.58	3.55	1.21	2.08	0.21	199.92	[33]
(26) N-Acetyl caprolactam	-0.80	3.20	3.18	2.12	0.20	189.89	[34]
(27) Succinimide	-0.80	3.28	1.95	2.02	0.25	110.08	[20]
(28) 2-Vinylpyridine	-1.47	2.62	2.03	2.29	0.12	140.84	[20]
(29) 2-Cyanofuran	-1.57	2.81	4.75	2.04	0.20	112.84	[35]
(30) Methyl cinnamate	-2.05	2.33	2.79	2.36	0.27	202.65	[20]
(31) Vinyl ethylene sulfite	-0.96	3.44	3.63	2.12	0.21	141.96	[36]
(32) Chloroethylene carbonate	-0.43	4.18	4.67	2.02	0.20	114.92	[20]
Ethylene carbonate (EC)	0.81	4.53	5.34	2.24	0.29	92.75	
Propylene carbonate (PC)	0.84	4.50	5.52	2.32	0.31	113.37	

supporting the reliability of our $\text{BE}(\text{Li}^+)$ results in Table 1. It should be noted that the binding energies in Table 2 are marginally affected by the use of different dielectric constant values ranging from 10 to 50 in the CPCM calculations, as shown in Table 3; this implies that the results and discussion are effective over a wide range of compositions of commercial battery electrolytes used in LIBs.

Why is a low Li^+ binding affinity preferred in SEI-forming additives? Recently, Sagane et al. [51] and Xu et al. [52] demonstrated through various experiments that the desolvation process, that is, the stripping of the solvation sheath of Li^+ , is the major energy-consuming step in LIBs. Moreover, Kobayashi and Uchimoto [53] proposed that the desolvation process of Li^+ involves the following steps: (i) partial desolvation, (ii) anion formation on the electrode, (iii) surface diffusion, and (iv) loss of the remaining solvents. It is considered that the weak binding of the additive with Li^+ ions facilitates the reaction steps (i) and (ii), thereby accelerating the overall desolvation step [54].

Finally, Halls and Tasaki [4] proposed an additive candidate (3353 in Ref. [4]) with high electron affinity, low η , and high μ

Table 2
Calculated Li^+ binding energies (in eV) of $\text{Li}^+(\text{EC})_2(\text{additive})$ model in gas and solution phases.

$\text{Li}^+(\text{EC})_2(\text{additive})$	Li^+ binding energy	
	Gas	Solution
Vinylene carbonate (1)	0.93	0.18
Maleic anhydride (7)	0.77	0.07
Ethylene carbonate (EC)	1.04	0.23

values based on their PM3 calculations. The DFT calculations in the present study agree with these values and confirm that the additive has a low Li^+ binding affinity (0.21 eV) with respect to EC (0.29 eV), and thereby supports the promising viability of the SEI-forming additive.

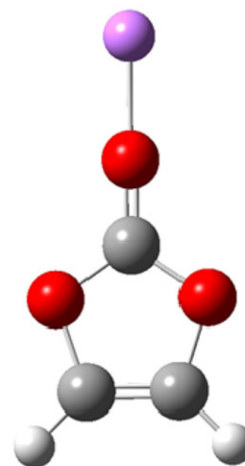
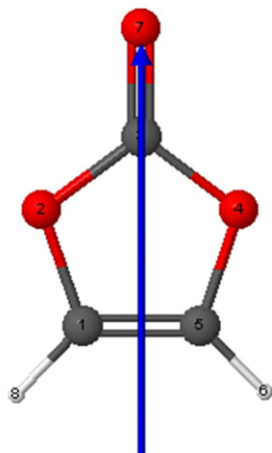
The low Li^+ binding affinity of the SEI-forming additives is not the only indicator of better performance. Other factors, such as fast reduction and the physical properties of the SEI layer [55,56], are also important for successful SEI formation. It is evident, however, that the Li^+ binding affinity is strongly connected with the SEI-forming properties of additives in LIBs. Consequently, it is proposed that the Li^+ binding affinity ($\text{BE}(\text{Li}^+)_{\text{sol}}$) should be included as a screening factor in the computational screening process for obtaining promising additives to accelerate the discovery and development of additives for enhancing battery performance.

Table 3
 Li^+ binding energies (in eV) using different dielectric constants for $\text{Li}^+(\text{EC})_2(\text{additive})$ systems.

ϵ	Li^+ binding energy		
	1	7	EC
10.0	0.23	0.12	0.29
20.0	0.20	0.08	0.25
31.9	0.18	0.07	0.23
40.0	0.18	0.07	0.23
50.0	0.17	0.06	0.22

Vinylene carbonate (1), maleic anhydride (7), and ethylene carbonate (EC).

(a) vinylene carbonate (1)



(b) maleic anhydride (7)

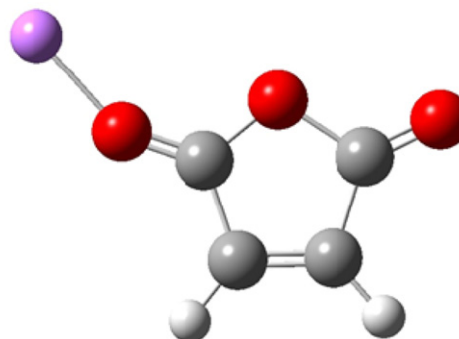
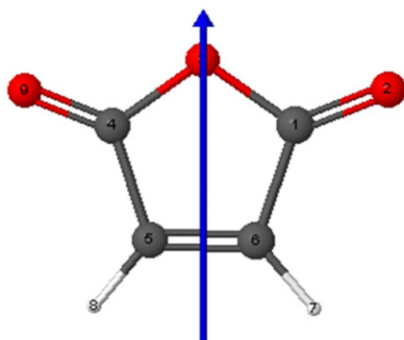


Fig. 2. Optimized structures with or without a Li^+ ion: (a) vinylene carbonate (1) and (b) maleic anhydride (7). Arrows denote molecular dipole moments.

4. Conclusions

The LUMO, η , μ and $\text{BE}(\text{Li}^+)$ values of 32 additives have been examined to understand the characteristics of SEI-forming additives in LIBs. The calculations confirm that both the LUMO and η values are critical indicators of suitable SEI formation. The μ values of the additives are generally smaller than those of the widely used solvents EC and PC. It is found that the low Li-ion binding affinity is an important characteristic for SEI-forming additives. It is proposed that Li^+ binding affinity can be used as a screening factor in the computational screening process for obtaining promising additives. It is anticipated that this work will help researchers using computational screening to search for novel additives more effectively.

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