



# High-throughput quantum chemistry and virtual screening for lithium ion battery electrolyte additives

Mathew D. Halls<sup>a,\*</sup>, Ken Tasaki<sup>b</sup>

<sup>a</sup> Materials Science Division, Accelrys Inc., San Diego, CA 92121, United States

<sup>b</sup> Technology Research Division, Mitsubishi Chemical Inc., Redondo Beach, CA 90277, United States

## ARTICLE INFO

### Article history:

Received 31 July 2009

Received in revised form

11 September 2009

Accepted 11 September 2009

Available online 20 September 2009

### Keywords:

Lithium ion battery

Electrolyte additive

SEI formation

Quantum chemistry

## ABSTRACT

Advances in the stability and efficiency of electronic structure codes along with the increased performance of commodity computing resources has enabled the automated high-throughput quantum chemical analysis of materials structure libraries containing thousands of structures. This allows the computational screening of a materials design space to identify lead systems and estimate critical structure–property limits which should prove an invaluable tool in informing experimental discovery and development efforts. Here this approach is illustrated for lithium ion battery additives. An additive library consisting of 7381 structures was generated, based on fluoro- and alkyl-derivatized ethylene carbonate (EC). Molecular properties (e.g. LUMO, EA,  $\mu$  and  $\eta$ ) were computed for each structure using the PM3 semiempirical method. The resulting lithium battery additive library was then analyzed and screened to determine the suitability of the additives, based on properties correlated with performance as a reductive additive for battery electrolyte formulations.

© 2009 Elsevier B.V. All rights reserved.

## 1. Introduction

For lithium ion batteries, the electrolyte typically consists of one or more lithium salts dissolved in an aprotic solvent, often with at least one additional functional additive. Additives are included in electrolyte formulations to perform specific functions. A common function is to enhance electrode stability by facilitating the formation of the solid/electrolyte interface (SEI) layer. Electrolyte additives include cyclic carbonates, such as vinylene carbonate, vinyl ethylene carbonate, fluoro ethylene carbonate, and alkyl carbonate derivatives [1–3]. Recently, fluorinated additives have attracted attention in light of their ability to increase the chemical stability of electrolytes against high potentials [4]. The discovery and development of additives to increase battery performance is of critical importance, yet such efforts often involve a hit-or-miss empirical investigative process. The computational screening of chemical design space for promising additives has the potential to greatly accelerate this time consuming process. Furthermore, theoretical insight into the effects of fluorination and or alkylation on fundamental anode SEI additive properties would be useful in guiding experimental efforts.

The use of virtual structure libraries for computational screening to identify lead systems for further investigation has become a

standard approach in drug design. [5,6] Transferring this paradigm to challenges in material science is a recent possibility due to advances in the speed of computational resources and the efficiency and stability of materials modeling packages. In particular, electronic structure codes are extremely robust for standard types of analyses, usually requiring no user intervention once the physical system and parameters have been set and the calculation initiated. This makes it possible for individual calculation steps to be executed in sequence comprising a high-throughput quantum chemistry workflow, in which material systems of varying structure and composition are analyzed in an automated fashion with the results collected in a growing data record. This record can then be sorted and mined to identify lead candidates and establish critical structure–property limits within a given chemical design space. To-date, only a small number of studies have been reported in which quantum chemical calculations are used in a high-throughput fashion to compute properties and screen for optimal materials solutions. [7,8–11] However, with time high-throughput computational screening will become central to advanced materials research.

In the current work, high-throughput quantum chemistry and virtual screening is demonstrated to explore the effects of fluorination and alkylation on the properties of ethylene carbonate (EC), as the reference. A virtual structure library based on derivatized EC is enumerated and each structure is analyzed using quantum chemical methods. The resulting database consisting of 7381 structures is then analyzed to determine variable limitations and identify sys-

\* Corresponding author. Tel.: +1 858 822 9998; fax: +1 858 799 5100.

E-mail addresses: [mhalls@mhalls.com](mailto:mhalls@mhalls.com), [mhalls@accelrys.com](mailto:mhalls@accelrys.com) (M.D. Halls).

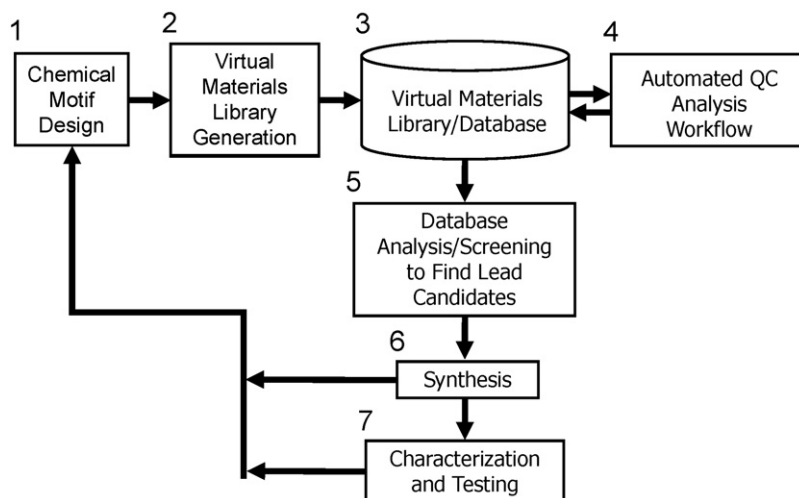


Fig. 1. Materials discovery and optimization scheme employing high-throughput quantum chemical analyses and virtual material screening.

tems with properties characteristic of effective graphite anode SEI additives.

## 2. Methods

The results summarized in this work were obtained using the VAMP semiempirical electronic structure package [12]. Calculations were carried out using the PM3 semiempirical Hamiltonian [13]. The sequence of geometry optimization and single-point energy calculations for neutral and charged species to obtain the HOMO and LUMO energies, vertical ionization potentials, electron affinities, and chemical hardness was captured in a workflow pipeline using the Materials Component Collection 4.4 within Pipeline Pilot (Version 7.5) [14]. The Pipeline Pilot workflow platform allowed the generation and automated quantum chemical analysis of an anode SEI additive structure library containing 7381 stereochemically unique structures. The SEI additive library was generated using an exhaustive combinatorial R-group enumeration scheme (array-based enumeration). Both the electronic structure code, VAMP, and the workflow platform, Pipeline Pilot, are commercially available from Accelrys, Inc.

## 3. Results and discussion

High-throughput quantum chemical analysis and virtual screening promises to revolutionize materials discovery for advanced applications such as lithium ion batteries. The process involves the generation of materials structure libraries (molecules, ensembles, surfaces), followed by high-throughput

quantum chemical analysis to compute key intrinsic properties and reaction energetics directly related to battery component performance and compatibility. The resulting virtual materials database is a unique and powerful resource, allowing the identification of optimal structures/formulations to advise experimental efforts through data mining and screening of chemical design space in a manner similar to the scheme outlined in Fig. 1. In the current work, steps 1 through 5 of the computational materials screening workflow is illustrated for lithium ion battery additives.

Semiempirical electronic structure techniques enable the quantum mechanical prediction of geometry, electronic structure and fundamental molecular properties at a small fraction of the cost of traditional *ab initio* methods. The speed, versatility and established accuracy of these methods make them well suited for high-throughput quantum chemical analysis, in which hundreds to thousands of structures can be analyzed. In the present work the PM3 semiempirical Hamiltonian is used [13] which has been shown to be useful in predicting the reactivity of fluorinated structures [15] and the reduction behaviour of electrolyte components [16].

In lithium ion batteries utilizing a graphite anode, cyclic carbonates are often used as anode SEI additives. They are selected with the aim of controlling the chemistry at the anode/electrolyte interface. An SEI film is formed during the first charge cycle. The initiation step leading to anode SEI formation is electron transfer to the SEI forming species resulting in a concerted or multi-step decomposition reaction producing the passivating SEI layer at the graphite–electrolyte interface [3,17,18]. Therefore, an important requirement for electrolyte additives selected to protect the elec-

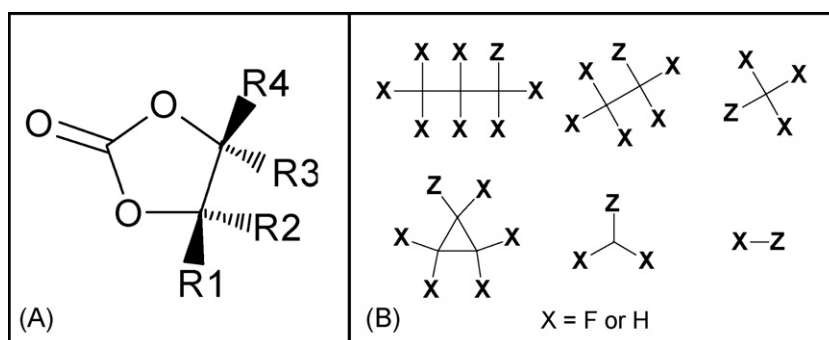


Fig. 2. Molecular core and R-group structures used to enumerate the alkyl- or fluoro-derivatized EC structure library: (A) ethylene carbonate (EC) core structure indicating the R1–R4 group positions and (B) the various alkyl R-group scaffolds with Z denoting the connection point and X = F or H.

**Table 1**

Ethylene carbonate (EC)-based additive library characterized in terms of relative property minimum (Min), maximum (Max), mean (Mean) and standard deviation (Std. dev.).

Relative property	n = 7381			
	Min	Max	Mean	Std. dev.
HOMO (eV)	-1.75	0.64	-0.56	0.46
LUMO (eV)	-3.42	0.27	-1.81	0.85
Ionization potential (IP) (eV)	-1.19	2.20	0.27	0.52
Electron affinity (EA) (eV)	-0.01	4.13	2.35	0.88
Dipole moment ( $\mu$ ) (D)	-4.70	2.81	-0.86	1.39
Polarizability ( $\alpha$ ) ( $\text{\AA}^3$ )	0.00	29.00	13.88	4.49
Chemical hardness ( $\eta$ ) (eV)	-1.69	0.02	-1.04	0.32

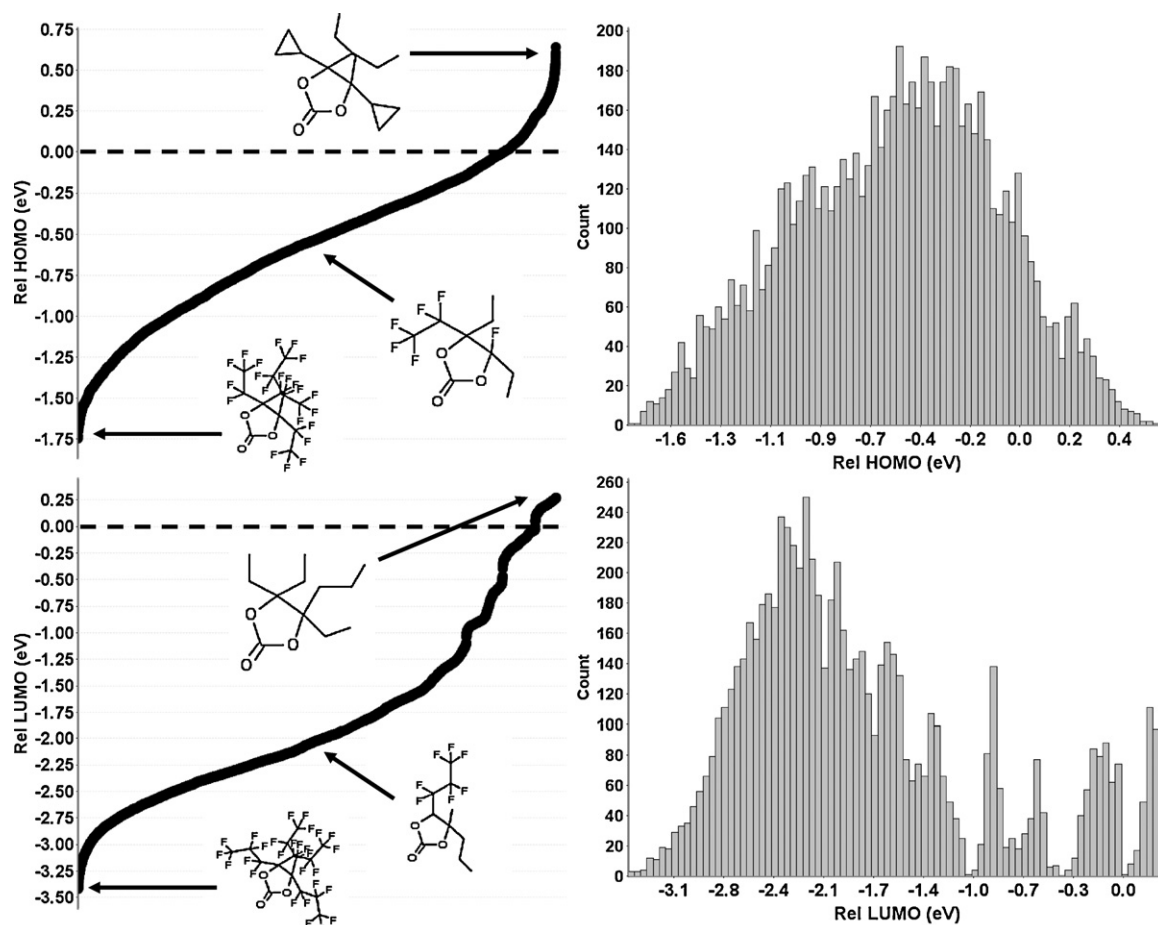
trolyte solvent from decomposition would be a higher reduction potential than the solvent. Chung et al. [16] have shown that trends in the lowest unoccupied molecular orbital (LUMO) calculated using semiempirical quantum chemical methods reflected the empirical reduction potentials for electrolyte components. This is in accordance with Koopman's theorem, in which the negative value of a system's LUMO energy is an approximation of its electron affinity [19]. Effective anode SEI additives should possess a low LUMO energy or a correspondingly high electron affinity (EA). An additional favorable characteristic for anode SEI additive selection is increased reactivity in order to facilitate good SEI formation. One measure of the relative reactivity of a series of related structures is their chemical hardness, defined by the following equation [20]:

$$\eta = \frac{IP_v - EA_v}{2}$$

where  $IP_v$  and  $EA_v$  correspond to the vertical ionization potential and electron affinity, respectively. Molecules with a large  $IP_v$  and low  $EA_v$  are less chemically active, i.e., they are chemically hard; therefore a small  $\eta$  would be a favorable feature of a SEI additive candidate. Additionally, an effective anode SEI additive may also possess a significant electric dipole moment ( $\mu$ ) since a larger value of  $\mu$  leads to stronger non-bonded interactions with  $Li^+$  to form stable lithium salts as SEI film components, though this may not always be a requirement.

To investigate the substituent effects on key properties, arising from the addition of alkyl- or fluoro-substituents to a base ethylene carbonate (EC) structure, a library of 7381 stereochemically unique additive structures was generated via an R-group substitution scheme. The chemical space is defined by exhaustively combining the EC core structure, shown in Fig. 2(A), with fluorine- and hydrogen-terminated alkyl R-groups shown in Fig. 2(B). For each of the R-groups shown in Fig. 2(B), the number of carbon atoms is  $\leq 3$ . Quantum chemical analysis of these structures allows the determination of property limits and variability of this focused chemistry for engineering EC-derived additives.

Using the PM3 level of theory, the relative molecular properties for each structure were computed as the difference from those computed for EC. The relative properties under examination are the HOMO and LUMO energies, vertical ionization potential ( $IP_v$ ), vertical electron affinity ( $EA_v$ ), chemical hardness ( $\eta$ ), dipole moment ( $\mu$ ) and mean electronic polarizability ( $\alpha$ ). The additive structure library relative property ranges, averages and standard deviations are presented in Table 1. To visualize the variation and distribution of the properties, ordered library plots and histograms for relative



**Fig. 3.** Ordered plots and histograms (left and right) for the relative HOMO and LUMO energies (top and bottom) for the EC-based additive library. Representative additive structures are shown, with their respective property values indicated.

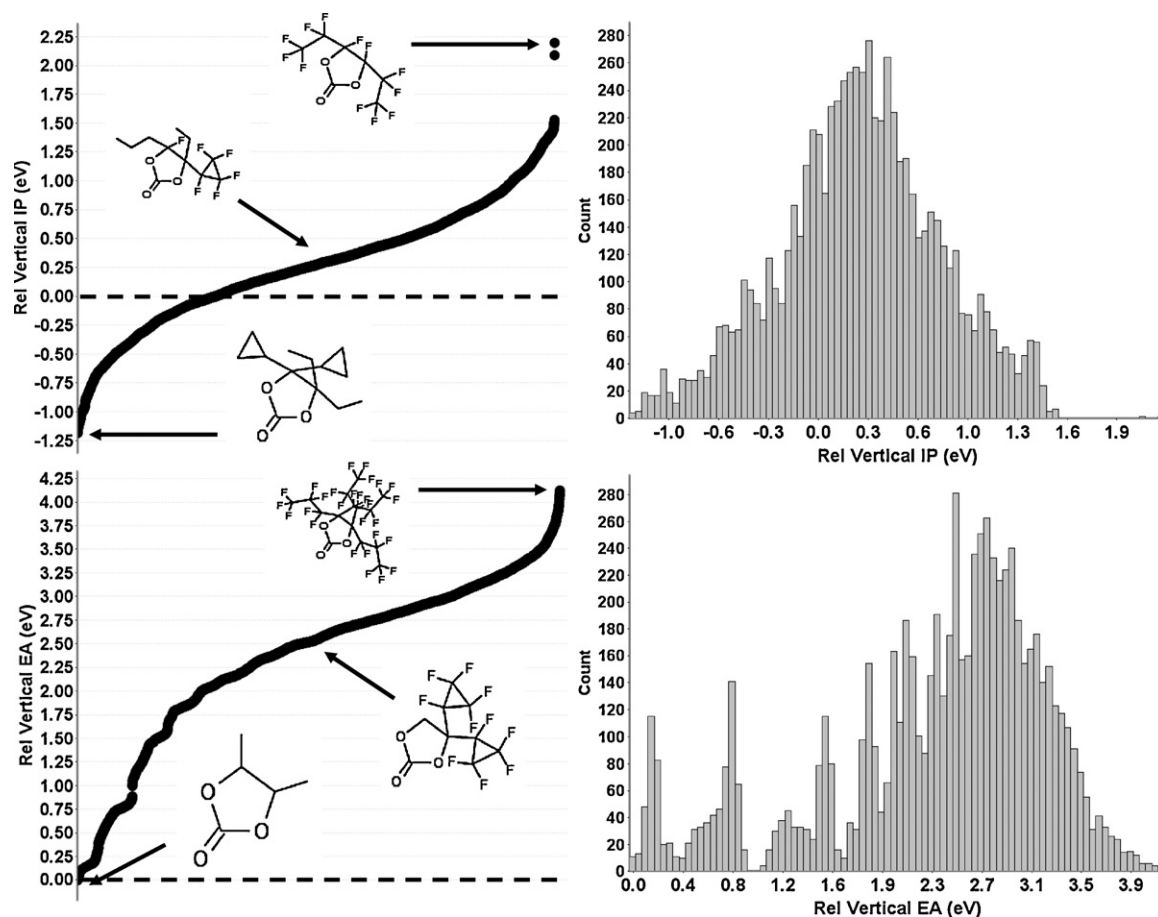


Fig. 4. Ordered plots and histograms (left and right) for the relative ionization potential (IP<sub>v</sub>) and electron affinity (EA<sub>v</sub>) (top and bottom) for the EC-based additive library. Representative additive structures are shown with their respective property values indicated.

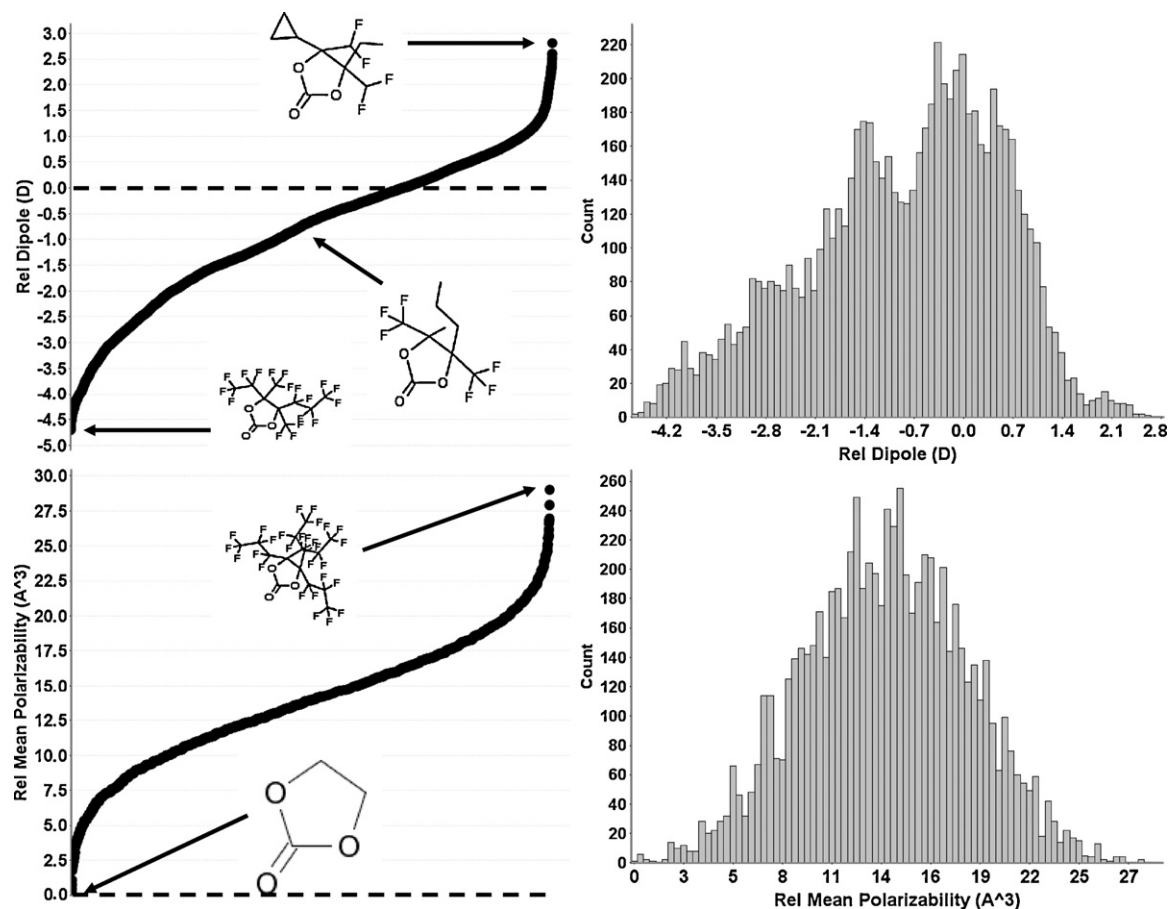
HOMO and LUMO, IP<sub>v</sub> and EA<sub>v</sub>,  $\mu$  and  $\alpha$ , and  $\eta$  are given in Figs. 3–6, respectively. In each of the figures, the left plot shows the variability in the property across the library by means of a scatter plot (XY) with the library structures ordered so that the relative property of interest is increasing. The ordered property plots are annotated to illustrate representative additive structures from the library. The plot on the right-side in each figure shows the property distribution across the library as a histogram of the calculated property. An immediate observation is that within the chemical space defined by the EC core and R-group chemistry shown in Fig. 2, all of the properties considered here vary nearly continuously over their range, with no properties showing discontinuous regions of property values.

Fig. 3 shows the variability and distribution of the relative HOMO and LUMO orbital energies with respect to those for EC across the structure library. As shown in the figure and in Table 1, the HOMO energy values range from  $-1.75$  eV below to  $0.64$  eV above the HOMO of EC. The library relative HOMO average and standard deviation is  $-0.56$  eV and  $0.46$  eV, respectively. The relative LUMO energies span from  $-3.42$  eV to  $0.27$  eV, with a mean and standard deviation of  $-1.81$  eV and  $0.85$  eV, respectively. For reductive anode SEI additives, a lower LUMO energy may be associated with facilitating SEI film production due to easier electron transfer at the graphite anode surface. As seen in Table 1 and Fig. 2, the majority of the library structures have a more favorable LUMO energy than EC. Closer inspection of the nature of the structures across the relative LUMO distribution indicates that those without fluorine have LUMO energies higher than that of EC. Since the LUMO is only an approximation to the true electron affinity, a more direct descriptor for additive suitability is the EA<sub>v</sub>.

The relative vertical ionization potential and electron affinity library plots and histograms are presented in Fig. 4. The relative IP<sub>v</sub> ranges from  $-1.19$  eV to  $2.20$  eV, with a library average of  $0.27$  eV and standard deviation of  $0.52$  eV. Relative values of EA<sub>v</sub> are positive with a maximum of  $4.13$  eV, mean of  $2.35$  eV and standard deviation of  $0.88$  eV. This indicates that all SEI additive library structures will be improved electron acceptors over EC. However, the effect of including fluorine in the molecular structure on EA<sub>v</sub> values is striking. The minimum and maximum relative EA<sub>v</sub> for fluorinated structures is  $0.39$  eV and  $4.13$  eV, respectively. This is greatly improved, compared to  $-0.01$  eV and  $0.43$  eV for purely alkylated-EC structures.

Two fundamental properties that affect the intermolecular interactions of electrolyte additives or co-solvents are the electric dipole moment and mean polarizability. The plots for  $\mu$  and  $\alpha$  are given in Fig. 5. Compared to the dipole moment of EC, the additive structure dipole moments vary by  $-4.70$  to  $2.81$  D. The library relative dipole moment mean and standard deviation are  $-0.86$  D and  $1.39$  D, respectively. A sizeable electric dipole results in a strong dipole–cation interaction with the lithium cations. In the library 2285 structures have dipole moments larger than that of EC. The molecular polarizability is related to the condensed phase dielectric constant. All the structures have increased polarizability compared to EC (up to  $+29.00 \text{ \AA}^3$ ), which is expected since all the structures have a more extended framework than the EC core.

Chemical hardness is related to the stability of a system, reflecting its capacity to undergo chemical reactions. From Table 1, the range of relative chemical hardness is  $1.71$  eV, with a minimal value of  $-1.69$  eV, a mean value of  $-1.04$  eV and a standard deviation of

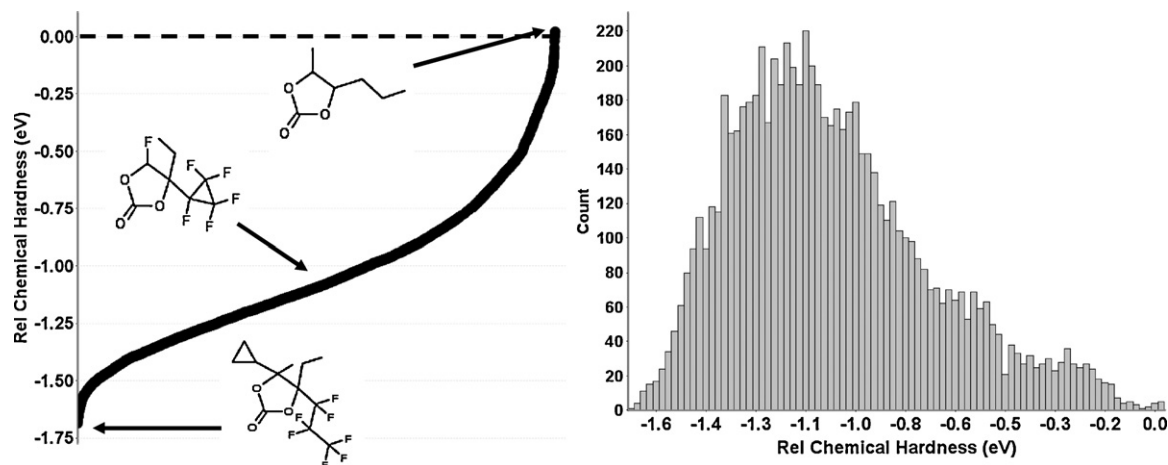


**Fig. 5.** Ordered plots and histograms (left and right) for the relative dipole moment ( $\mu$ ) and mean polarizability ( $\alpha$ ) (top and bottom) for the EC-based additive library. Representative additive structures are shown with their respective property values indicated.

0.32 eV. Fig. 6 presents the library relative chemical hardness plots. As seen in the figure, chemical derivatization by alkyl or fluorinated alkyl groups softens the system compared to EC, which is desirable for effective additives as it should relate to decreased stability. Here again fluorinated cyclic carbonates are more favorable as SEI additives, with a minimum hardness of  $-1.69$  eV compared to EC, which is 0.93 eV smaller than the lowest  $\eta$  for alkylated structures.

Overall, the addition of fluorinated substituents to the ethylene carbonate core substantially improves the molecular properties

that correlate with reductive SEI additive performance. The relative properties are predicted to vary with the number of fluorine atoms in the molecular structure. The average relative LUMO energy, electron affinity ( $EA_v$ ) and chemical hardness ( $\eta$ ) for structures having 1, 3 and 5 fluorines are  $-0.10$  eV,  $0.59$  eV,  $-0.45$  eV ( $n(F)=1$ ),  $-0.85$  eV,  $1.43$  eV,  $-0.75$  eV ( $n(F)=3$ ) and  $-1.51$  eV,  $2.05$  eV,  $-1.05$  eV ( $n(F)=5$ ), respectively. The LUMO,  $EA_v$  and  $\eta$  for structures with  $n(F) > 5$  are  $-2.27$  eV,  $2.82$  eV and  $-1.18$  eV, respectively.



**Fig. 6.** Ordered plot and histogram (left and right) for the relative chemical hardness ( $\eta$ ) for the EC-based additive library. Representative additive structures are shown with their respective property values indicated.

**Table 2**

Relative properties (molecular volume, HOMO, LUMO, dipole moment ( $\mu$ ), mean polarizability ( $\alpha$ ), vertical IP ( $IP_V$ ), vertical electron affinity ( $EA_V$ ) and chemical hardness ( $\eta$ )) with respect to ethylene carbonate (EC) values for butyl sultone (BS), propylene carbonate (PC), fluoroethylene carbonate (FEC) and structure 3353 computed at the PM3 level of theory.

Structure	Formula	MW	Rel. volume ( $\text{\AA}^3$ )	Rel. HOMO (eV)	Rel. LUMO (eV)	Rel. $\mu$ (D)	Rel. $\alpha$ ( $\text{\AA}^3$ )	Rel. $IP_V$ (eV)	Rel. $EA_V$ (eV)	Rel. $\eta$ (eV)
Butyl sultone (BS)	$C_4H_8SO_3$	138.19	84.03	0.68	-1.17	0.70	4.10	-0.72	1.57	-0.86
Propylene carbonate (PC)	$C_4H_6O_3$	102.09	12.35	0.09	0.06	0.26	1.76	-0.23	0.30	-0.26
Fluoro-EC (FEC)	$C_3H_3FO_3$	106.05	5.49	-0.26	-0.27	-0.41	0.18	0.16	0.42	-0.13
3353	$C_{12}H_{13}F_7O_3$	338.22	138.23	-0.17	-2.20	-0.46	16.89	-0.63	2.74	-1.69

Structure 3353 (shown in Fig. 7) is a Pareto-optimal candidate, simultaneously  $\uparrow$  ( $EA_V$  and  $\mu$ ) and  $\downarrow$   $\eta$ .

For a given materials application, finding exemplary structures involves simultaneously satisfying a number of target objectives, in this case based on the fundamental properties related to their anode SEI additive performance. Multi-objective solutions represent a trade-off between objectives, with one class being Pareto-optimal solutions [21]. Pareto-optimal solutions are defined as a set of solutions which are non-dominated, such that it is not possible to improve one property without making any other property worse [10,22].

As noted above, for reductive anode SEI additives, the major selection criterion is that the species be reduced at the anode before the other electrolyte components in the system. Ease of reduction is correlated with the molecular electron affinity,  $EA_V$ . It follows that in selecting for noteworthy SEI structures maximizing  $EA_V$  is a key objective. A second objective in selecting SEI additives may be to minimize the chemical hardness,  $\eta$ , which will correlate to a more reactive species. The electric dipole of the system,  $\mu$ , will determine the strength of the electrostatic interactions between the additive and  $Li^+$ . Screening the 7381 EC-based structures for the Pareto-optimal solutions that maximize  $EA_V$  and  $\mu$ , while simultaneously minimizing  $\eta$  results in a set of structures that represent the best compromise in terms of property trade-off. An exemplary structure from the Pareto-optimal set is additive 3353 from the library, whose properties are given in Table 2 and its molecular structure is shown in Fig. 7. This structure has  $R_1 = CH_3$ ,  $R_2 = C_3H_5$ ,  $R_3 = C_3F_7$ ,  $R_4 = C_2H_5$  attached to the EC core. The  $EA_V$  and  $\eta$  for the structure 3353 is computed to be 2.74 eV above and 1.69 eV below those of the EC reference.

To gain confidence in the SEI additive screening approach presented here, the PM3 computed relative properties for butyl sultone (BS), propylene carbonate (PC) and fluoroethylene carbonate (FEC) are also presented in Table 2 for comparison. Experimentally, butyl sultone (BS) has been reported to be a highly effective graphite anode SEI forming additive in electrolyte formulations involving propylene carbonate (PC) as a co-solvent. [23] The use of BS as an

electrolyte additive overcame performance issues seen with the application of PC as a co-solvent, such as the loss of discharge capacity and decrease of cycling stability. BS has a higher reduction potential than PC, thus undergoing reductive decomposition faster and forming a passivating SEI film that suppresses subsequent PC decomposition. A comparison of the computed properties for BS and PC listed in Table 2 supports the good performance of BS as an SEI additive. BS is predicted to be more easily reduced than PC, having an electron affinity 1.27 eV larger than that computed for PC. The chemical hardness of BS is 0.60 eV lower than that of PC, suggesting it would be more reactive, facilitating SEI formation.

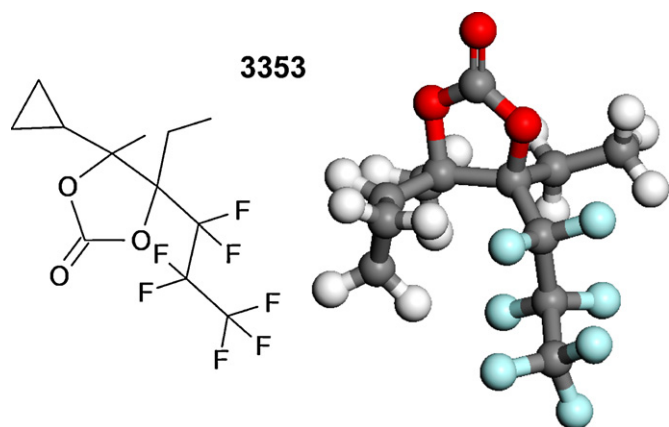
Fluoroethylene carbonate (FEC) has also been used experimentally as an SEI additive in electrolytes for lithium ion batteries [24,25]. Using an ethylene carbonate (EC) containing solvent, the addition of FEC at 10% and 30% levels, shifted the onset of SEI formation to higher potentials by +0.25 eV and +0.38 eV, compared to 0.4 eV for the base solvent vs.  $Li/Li^+$ . The relative properties for FEC listed in Table 2 provide a rationalization for this observation. As seen there, FEC has a higher electron affinity (+0.42 eV) and a lower chemical hardness (-0.13 eV) than EC, suggesting superior SEI forming behaviour.

The results presented here introduce a new and powerful approach for exploring the property limits of structural motifs for lithium battery electrolyte additives. High-throughput computational screening has the potential to dramatically reduce the time and effort for evaluating new synthetic directions for anode SEI formation additives, given that the time required to calculate the key molecular properties needed for relative screening was less than ca. 20 s per structure. Such screening studies can help reduce costs by informing experimental efforts allowing them to focus on the most productive candidates. Our findings suggest the improved performance for additives incorporating fluorine and are consistent with the limited experimental reports of fluorinated-SEI additives reported in the literature [2,24,25,26].

The prospect of automating complex material modeling workflows to explore formulation and chemical design space has the potential to rapidly accelerate materials discovery, analysis and optimization. This approach is applicable to material systems ranging from discrete molecules and clusters, to periodics such as surfaces and crystals. In addition to identifying specific lead candidates to pursue experimentally, when analyzed using data mining and reduction techniques, the resulting aggregate of data from high-throughput modeling studies will reveal structure-property trends and underlying physical patterns.

#### 4. Conclusions

The use of high-throughput quantum chemistry to analyze and screen a materials structure library representing a well defined chemical design space has been applied to fluoro- and alkyl-derivatized ethylene carbonate (EC). The fundamental properties of these systems were evaluated as graphite anode SEI additives in lithium ion battery electrolyte formulations. The effect of fluorination leads to a maximum electron affinity across the library



**Fig. 7.** Molecular structure for EC-based additive candidate 3353 representing a Pareto-optimal structure, simultaneously  $\uparrow$  ( $EA_V$  and  $\mu$ ) and  $\downarrow$   $\eta$ .

of 4.13 eV, compared to alkylation leading to a maximum value of only 0.43 eV, relative to EC. A large electron affinity is a critical requirement for improved additive activity. The library was screened to identify an exemplary Pareto-optimal additive structure, which represents a promising lead for future investigation. We propose our approach as a new screening tool in order to facilitate the development of additives for lithium ion battery electrolytes.

### Acknowledgements

Support from Accelrys, Inc. and Mitsubishi Chemical, Inc. is gratefully acknowledged. Also, the authors thank the Hewlett–Packard Corporation for providing computational resources to enable this work.

### References

- [1] M.C. Smart, B.V. Ratnakumara, V.S. Ryan-Mowreya, S. Surampudi, G.K.S. Prakash, J. Hub, I. Cheung, J. Power Sources 119–121 (2003) 359.
- [2] S.S. Zhang, J. Power Sources 162 (2006) 1379.
- [3] K. Xu, Chem. Rev. 104 (2004) 4303.
- [4] D. Howell, Progress Report for Energy Storage Research and Development, Department of Energy, 2009, January.
- [5] T.J. Marrone, J.M. Briggs, J.A. McCammon, Ann. Rev. Pharmacol. Toxicol. 37 (1997) 71.
- [6] R.D. Brown, S. Varma-O'Brien, D. Rogers, QSAR Comb. Sci. 25 (2006) 1181.
- [7] J.A. Hageman, J.A. Westerhuis, H.-W. Fruhauf, G. Rothenberg, Adv. Synth. Catal. 348 (2006) 361.
- [8] D. Morgan, G. Ceder, S. Curtarolo, Meas. Sci. Technol. 16 (2005) 296.
- [9] J. Greeley, T.F. Jaramillo, J. Bonde, I. Chorkendorff, J.K. Nørskov, Nat. Mater. 5 (2006) 909.
- [10] T. Bligaard, G.H. Jóhannesson, A.V. Ruban, H.L. Skriver, K.W. Jacobsen, J.K. Nørskov, Appl. Phys. Lett. 83 (2003) 4527.
- [11] T. Bligaard, J.K. Nørskov, Electrochim. Acta 52 (2007) 5512.
- [12] T. Clark, A. Alex, B. Beck, F. Burkhardt, J. Chandrasekhar, P. Gedeck, A. Horn, M. Hutter, B. Martin, G. Rauhut, W. Sauer, T. Schindler, T. Steinke, VAMP: Version 10.0, Erlangen, 2003.
- [13] J.J.P. Stewart, J. Comp. Chem. 10 (1989) 209.
- [14] S. Varma-O'Brien, F.K. Brown, A. LeBeau, R.D. Brown, Curr. Comput. Aided Drug Des. 4 (2008) 13.
- [15] C.A. Heaton, A.K. Miller, R.L. Powell, J. Fluorine Chem. 107 (2001) 1.
- [16] G.-G. Chung, H.-J. Kim, S.-I. Yu, S.-H. Jan, J.-W. Choi, M.-H. Kim, J. Electrochem. Soc. 147 (2000) 4291.
- [17] X. Zhang, R. Kostecki, T.J. Richardson, J.K. Pugh, P.N. Ross, J. Electrochem. Soc. 148 (2001) A1341.
- [18] A.N. Dey, Thin Solid Films 43 (1977) 131.
- [19] T. Koopmans, Physica 1 (1933) 104.
- [20] R.G. Pearson, J. Org. Chem. 54 (1989) 1423.
- [21] V. Pareto, Manuale di Economia Politica, Societa Editrice Libreria, Milano, 1906, translated to English as: V. Pareto, Manual of Political Economy, Macmillan, New York (1971).
- [22] M.P. Andersson, T. Bligaard, A. Kustov, K.E. Larsen, J. Greeley, T. Johannessen, C.H. Christensen, J.K. Nørskov, J. Catal. 239 (2006) 501.
- [23] M.Q. Xu, W.S. Li, X.X. Zuo, J.S. Liu, X. Xu, J. Power Sources 174 (2007) 705.
- [24] R. McMillan, H. Slegr, Z.X. Shu, W. Wang, J. Power Sources 81–82 (1999) 20.
- [25] N.-S. Choi, K.H. Yew, K.Y. Lee, M. Sung, H. Kim, S.-S. Kim, J. Power Sources 161 (2006) 1254.
- [26] M. Kobayashi, T. Inoguchi, T. Iida, T. Tanioka, H. Kumase, Y. Fukai, J. Fluorine Chem. 120 (2003) 105.