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Successes and failures predicting the solubility of solid electrolyte interphase (SEI) species

Johanna Timhagen [a], Vigneshwaran Thangavel [a,b], Juan Forero-Saboya [c,d], Jonathan Weidow [a], Patrik Johansson [a,e,f,*]

[a] *Department of Physics, Chalmers University of Technology, 412 96, Gothenburg, Sweden*
[b] *Present address: Scania CV AB, 151 87, Södertälje, Sweden*
[c] *Chimie du Solide et de l'Energie, CNRS UMR 8260, Collège de France, 75231 Paris, France*
[d] *Present address: Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA*
[e] *ALISTORE-European Research Institute, CNRS FR 3104, Hub de l'Energie, 80039 Amiens, France*
[f] *Department of Chemistry – Ångström, Uppsala University, 751 21 Uppsala, Sweden*

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ABSTRACT

The stability of the solid electrolyte interphase (SEI) is crucial for the cycle-life and safety of modern rechargeable batteries. The SEI is most often addressed by electrochemical and advanced surface characterization methods. A less trodden path is the solubility of the very species making up the SEI – a fundamental property that can be addressed both experimentally and computationally. Herein promises and problems of solubility assessments are highlighted, including successes and failures and how to possibly overcome them. Specifically, we experimentally contrast literature data *vs.* inductively coupled plasma mass spectrometry, and computationally we use a combination of density functional theory and statistical mechanics. Proof-of-concept is made for a few alkali and alkali earth metal, *i.e.* Li/Na/Mg/Ca, inorganic salts, but it can easily be expanded to *e.g.* organic species. Overall, experimentally determined solubilities are laden with large uncertainties and correlate only fairly with calculated solubilities. Deviations are especially pronounced for Mg and Ca-salts. Pushing this route further to create a general tool to assist in the very design of more stable SEIs, by finding and predicting non-soluble species for current and next generation battery technologies, is most probably viable, but both the experimental and the computational approaches need to be refined.

1. Introduction

Today's advanced rechargeable batteries, such as lithium-ion batteries (LIBs) and sodium-ion batteries (SIBs), have anodes, typically graphite and hard carbon, respectively, that operate well below the reduction potentials of the electrolytes employed [1]. This is also true for various proposed next generation battery (NGB) technologies, based on silicon conversion/alloying anodes [2] or lithium metal anodes [3], as well as other metal anodes, such as magnesium or calcium [4]. Thus, the electrolytes will inevitably decompose, yet the decomposition products can form a passivation layer; a solid electrolyte interphase (SEI), which prevents further electrolyte decomposition and makes possible useful battery operation [5,6]. Conventionally, the stability of the SEI, which affects both battery cycle-life and safety [6], is addressed by electrochemical and advanced surface characterization methods, and is enhanced by electrolyte additives [7], SEI-formers, such as vinyl carbonate (VC) for LIBs [8], that reduce prior to or in conjunction/synergy with the salt(s) and solvent(s) – together creating what has been coined *functional electrolytes* [9]. The cell formation stage uses reduction reactions that from the functional electrolyte create species *suggested* to take part in forming the SEI, but their solubilities in the battery electrolyte/solvents ultimately determines if they actually will. Predicting solubilities of species in electrolytes, either by designed experiments or computational assessments, *e.g.* high-throughput screening, would be a most welcome tool to speed up the SEI R&D process, especially for NGBs.

Yet, as of today, studies of the resulting SEIs are quite numerous [6], but practical electrolyte solubility studies with SEI relevance are significantly scarcer. Experimentally, direct techniques to identify atoms and molecules, such as induction coupled plasma optical emission

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* Corresponding author.
E-mail address: patrik.johansson@kemi.uu.se (P. Johansson).

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spectroscopy (ICP-OES) [10] and atomic absorption spectroscopy (AAS) [11], have been applied, but much more common are indirect approaches where the SEI stability, and hence the SEI-species' solubilities, is inferred from electrochemical studies – both for LIBs and SIBs [12–15] and a few NGBs [16–19]. The fact that relatively few direct experimental efforts targeting solubility properties have been made is possibly connected with the many practical difficulties, alongside a battery community where SEI research has almost entirely been devoted to electrode surface rather than electrolyte studies [20,21].

In some contrast, direct computational studies of SEI-species' solubilities are easier to create; for example Tasaki et al. calculated the heat of dissolution of Li-salts in dimethyl carbonate (DMC) using classical molecular dynamics (MD) simulations [22] and Cheng et al. used *ab initio* MD (AIMD) to study the solubility of Li_2O_2 and Li_2O in dimethoxyethane (DME) and benchmarked these *vs.* density functional theory (DFT) and MP2 calculations [23]. Furthermore, Pabsch et al. predicted solubilities of various Na, K and Cs-salts in three solvents, using electrolyte perturbed-chain statistical associating fluid theory (ePC-SAFT) [24]. These studies are however few and very specific to a few salts and solvents – no generic framework or route has been presented or even attempted to be created, why we are far from having any general and predictive model useful across different battery chemistries and designs.

Trying to partly remedy this, we here address the solubilities of the inorganic SEI species that are simple salts, in both water, propylene carbonate (PC), and also DMC as solvents. We do it experimentally by literature data and by inductively coupled plasma mass spectrometry (ICP-MS), and computationally by proposing a modelling route for assessing these prospective SEI-species' solubilities based on using the conductor-like screening model for real solvents (COSMO-RS), which uses a quantum chemical continuum solvation model [25] and statistical thermodynamics to predict properties of liquids from their molecular constituents [26–28]. COSMO-RS has previously been used to screen battery electrolyte solvents based on calculating properties such as boiling/flash points, pK_as, electrochemical stability windows, *etc* [29, 30]. Recently one of us has applied COSMO-RS to model solubilities of elemental sulfur and polysulfides for Li-S batteries [31–33], as well as Ca-salts for calcium batteries [34].

Combining all the above we can hopefully assess how much of the work-flow and know-how already gained can be transferred to the task of predicting the solubility of prospective SEI species and by successes and failures identify promises and problems. In the end, this should lead not only to a generally applicable tool/route, but also to a fast and inexpensive way to predict/screen the stability of any SEI, based on proposed species.

Herein we first make a rather straightforward comparison between experimental and calculated solubilities in water. Second, we move, by different correlations and approaches, especially for the non-Li-salts, to solubilities in PC and DMC. Finally, we conclude by summarizing the problems and failures as well as the promises and successes, and how to possibly overcome the remaining hurdles. Overall, we focus first hand on qualitative agreement, second hand on semi-quantitative agreement, and strive to provide simple and intuitive visualizations.

2. Experimental and computational

2.1. Solution preparation and experimental solubilities

We used a set of twelve small and simple inorganic alkali and alkali earth salts, built from four different cations and six different anions: Li_2CO_3, LiCl, LiF, LiOH, $LiNO_3$, Na_2CO_3, NaF, NaHCOO, $CaCO_3$, CaF_2, $MgCO_3$ and MgF_2 (Table S1). The salts were all dried at 50 °C under vacuum overnight. The PC solutions were prepared as follows: 120 mg of salt and 4 mL of dry PC were stirred using a magnetic stirrer, whereby cloudy solutions were obtained in all cases. The suspensions were filtered using PTFE syringe filters (0.2 μm) to obtain completely clear solutions. Subsequently, the PC was completely removed by vacuum distillation and the residual solid, barely present in some cases, was completely dissolved in 2 wt. % $HNO_{3(aq.)}$ and the resulting solution analyzed by ICP-MS using a Nexion 2000 instrument (Perkin Elmer). In the case of aqueous systems, saturated solutions were prepared inside a temperature-regulated chamber (25 °C) before filtering, diluting and analyzing them the exact same way. For DMC solubilities we strictly use literature data.

2.2. Differential scanning calorimetry (DSC)

The thermal property data needed as input to the COSMO-RS calculations (see below), *i.e.* the melting temperature (T_m) and the enthalpy of fusion (ΔH_{fus}) of the salts, were mainly taken from the literature [35–38]. The few additional experiments (Fig. S1, Table S1) needed were performed on a DSC250 (TA Instruments) using a scan rate of 2 K/min under flowing He gas and 5–7 mg of salt in sealed Al pans. For tests above the salt decomposition temperatures the pans had a pinhole to release any gas formed.

2.3. DFT and COSMO-RS calculations

Optimized molecular geometries were generated by DFT calculations using the Gaussian 16 suite [42], the PB86 functional [39,40] and the TZVP basis set [41], first in gas phase and then adding the conductor-like self-consistent reaction field (SCRF) COSMO ($\varepsilon=\infty$) [25] to implicitly account for solvent effects. The subsequent COSMO-RS calculations to create COSMO-files, that contain the σ-surfaces of the species, used the BP_TZVP_21 parameterization in COSMOtherm [43], and absolute solubilities were calculated using the solid-liquid equilibrium (SLE) method [28].

One intrinsic problem of COSMO-RS is that it handles hard cations, such as Li^+ and Mg^{2+}, but also small anions, such as F^-, less favorably. This is due to their high polarization charge densities and thereby very narrow σ-profiles (Fig. 1), which leads to problems not the least for solubility calculations [44]. A remedy is to use explicitly solvated ions [45–47], which have much broader σ-profiles, *e.g.* $[Li(S)_4]^+$ for $S = H_2O$ or PC in Fig. 1, that most often overlap with the σ-profiles of the electrolyte solvents. Indeed, without this remedy no solubilities were at all possible to calculate for LiF and CaF_2.

The salt solubilities were subsequently calculated using:

$$x_i^{bs} = \frac{x_i^{ss}}{1 + n_s x_i^{ss}} \tag{4}$$

where x_i^{bs} and x_i^{ss} are the mole fractions of the "bare" ions and solvates, respectively, and n_s is the number of solvent molecules in the solvate (Table S1).

While neither H_2O nor PC has more than one conformer, and thus are straightforward to calculate optimized geometries of, DMC has three stable conformers, *i.e. cis-cis, cis-trans*, and *trans-trans.* As these all are able to solvate cations [48,49], they were all evaluated via the COSMO*conf* tool [39,40]. This rendered *cis-cis* the most stable conformer (Table S2), whereas the stability of the *cis-trans* conformer increased upon cation interaction, in agreement with experimental Raman spectroscopy data [49]. Hence both the *cis-cis* and *cis-trans* conformers of DMC were used in the salt solubility calculations.

3. Results and discussion

3.1. Solubility in water

The solubility in water is readily available in the literature for all our salts, but to assess the quality of the experimental data we also add our own solubility data (Table S1). The first thing notable is the *ca.* two orders of magnitude difference in experimental solubilities, TS* *vs.* L*,

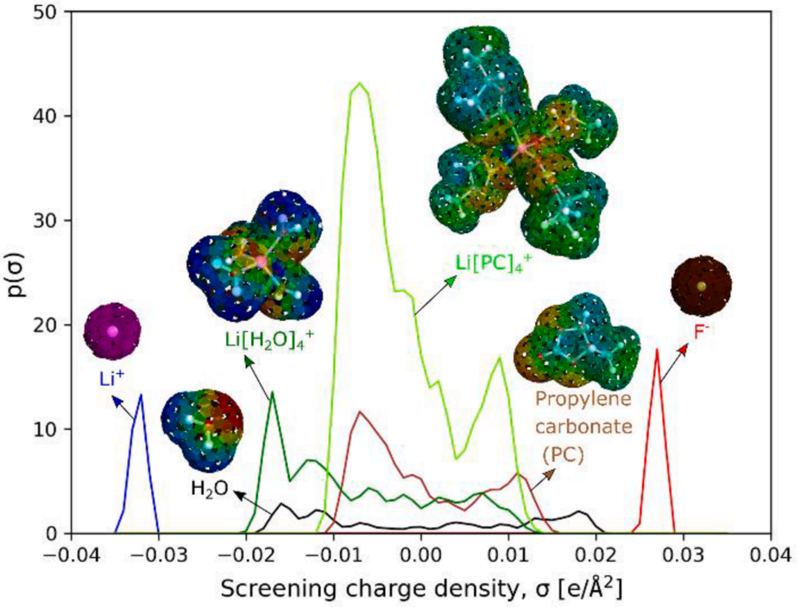

Fig. 1. *Examples of σ-profiles and σ-surfaces of ions, solvents, and solvates.*

more or less for all salts. This highlights the major difficulty obtaining accurate, trusted and error-free experimental solubility data. While we very carefully dried all salts prior to our experiments, which could render the (possibly more correct) lower solubility values for the TS* data set – little is usually noted on the drying of the salts in the literature, *i.e.* for the L* data set. However, admittedly many other factors may play a role in the actual values obtained.

Turning to the comparison with the COSMO-RS modelling, this approach as much of the development of computational approaches to model solubility in general, has been made with aqueous systems in mind. Considering this, as well as the above problems, the correlation between experimental and computed solubilities using the root mean square deviation (RMSD) as measure, renders the L* data a RMSD=1.02 and the TS* data a RMSD=1.88 (Fig. 2).

From the visualization, we intuitively find that for the monovalent species the agreement in general is much better for the L* data, but that for the divalent cation salts with the very lowest solubilities, *i.e.* $CaCO_3$, $MgCO_3$, and MgF_2, the TS* data are in better agreement. Yet, given the very large uncertainty in the experimental data it is close to impossible to unambiguously validate the computational approach.

3.2. *Solubility in PC and DMC*

For PC and DMC, more common LIB and also NGB solvents, the solubilities are in the literature reported only for a few lithium salts [4, 5], and not at all for Na, Mg, or Ca-salts. For the solubility in PC of the former (Table S1, Fig. 3 left) there is an even larger quantitative disagreement between the literature and our data than for the aqueous systems – up to four orders of magnitude. Again, we do not know the dryness of the salts in literature, and there is also the added issue of the PC used; if the PC used is not extra dry, the solubility would increase dramatically. Turning to the comparison with the computed solubilities, it is very clear that the L* data are much closer (RMSD=1.22) and the TS* data are quite much worse off (RMSD=4.86).

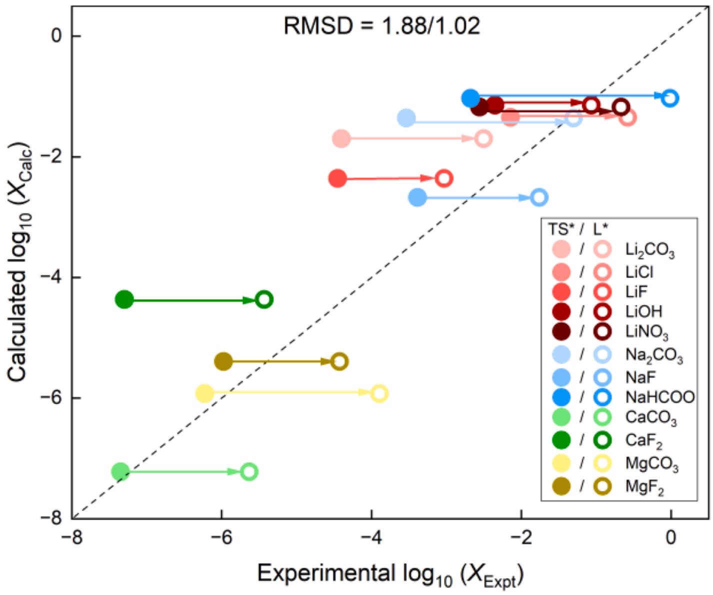

Fig. 2. Calculated and experimental solubilities (TS* = this study and L* = literature) in water.

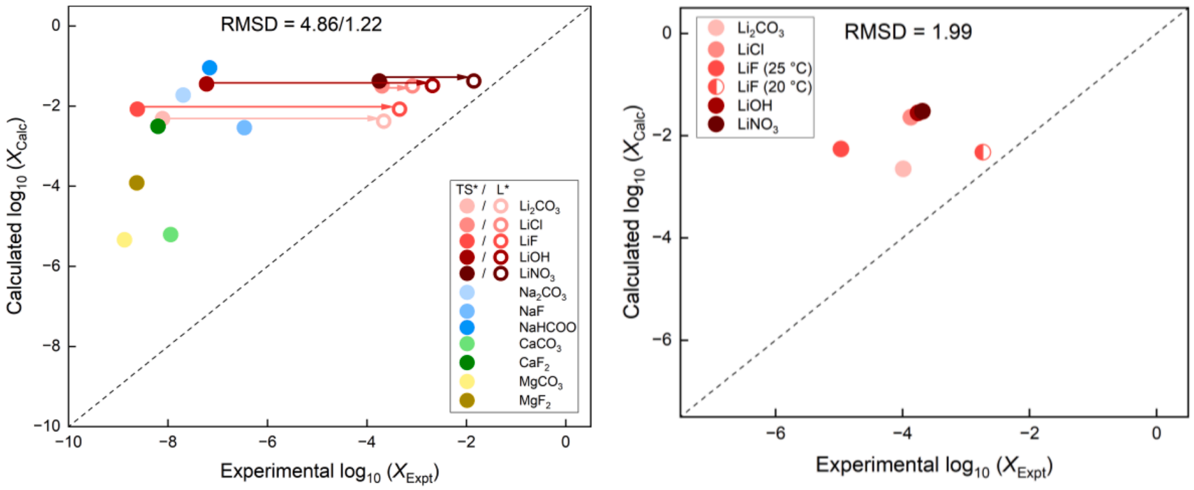

Fig. 3. Calculated and experimental solubilities in a) PC (left) and in b) DMC (right).

Qualitatively there are huge differences between the different Li-salts in the computed *vs.* experimental agreement also for the TS* data. For the computed solubilities we *e.g.* can note an one order of magnitude higher solubility of the corresponding Na-salts *vs.* Li-salts, which is what could be expected, and falling solubilities of the CO$_3$-salts as: Na>Li>Ca≈Mg and for the F-salts: Li>Na≈Ca>Mg.

Turning to the admittedly scarce DMC data (Table S1, Fig. 3 right), there is really no qualitative trend visible, but anyhow a notable observation is the very large difference in the literature for the solubility of LiF between Xin et al. [4] and Jones et al.[5]: 1.07×10^{-5} and $1.85 \times 10^{-3\ \mathrm{mol}}$ fractions, respectively, with the additional 5 °C negative difference as an add-on.

Qualitatively and quantitatively, it is clearly so that the computational approach seems to overestimate the salt solubilities both in PC and in DMC – all data points in Fig. 3 are found above the ideal line. As this was not the case for the aqueous systems and to overcome the fact that we have no solubility data for *non-Li-salts*, we here launch a comparative approach using the aqueous experimental L* data set (Fig. 4). A much better balance *vs.* the ideal line is this way obtained, with the notable exception of the large deviations for the divalent CO$_3$-salts.

4. Concluding remarks

One obvious large problem, and at least a partial cause of some failures we observe, is the large deviations obtained *vs.* experimental data and unreliable experimental data. The latter is perhaps surprising for such a fundamental property as solubility, but many factors contribute to the uncertainty, both materials and methodology. Yet, overall, the computed solubilities qualitatively, and sometimes even semi-quantitatively, somewhat match the experimentally observed data and trends. And as for the modelling approach, as we have already remedied the hard cation/anion problem of COSMO-RS via explicit solvation, one problem remaining could be that long-range interactions are not considered in COSMO-RS [44,46]. This may especially affect those salts where either one or both of the cations and anions are divalent – and we do see some large deviations for CO_3^{2-}, Mg^{2+} and Ca^{2+} salts. An additional problem is that no non-ideality, such as the Debye–Hückel effect, is considered, which also might be more pronounced for divalent chemistries. We thus have some particular difficult

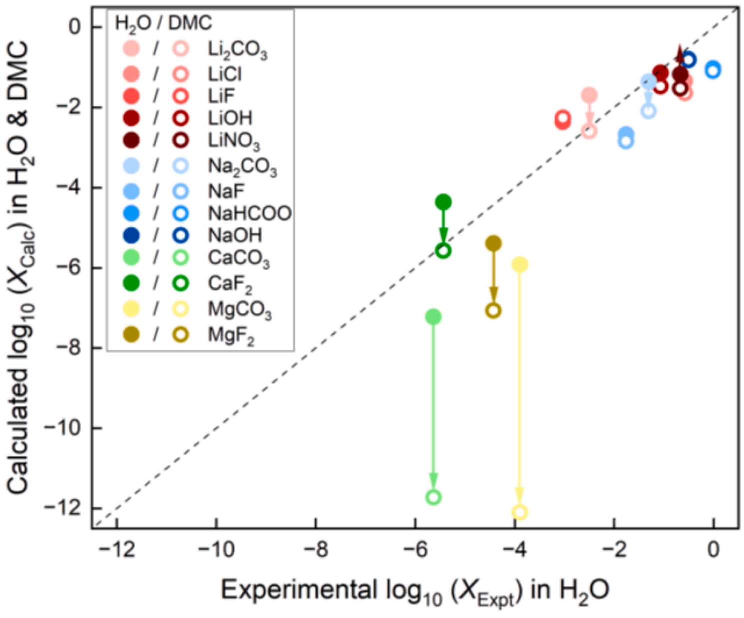

Fig. 4. Calculated solubilities in DMC and water *vs.* experimental solubilities in water.

cases included in our data set: salts with both divalent cations and anions, salts with the CO_3^{2-} divalent anion, and we should also add salts with the F^- anion – which is a species intrinsically difficult to treat correctly by DFT.

The main promise of the proposed approach, largely based on the tailored COSMO-RS methodology, is that it intrinsically offers the ability to predict the solubilities very resourcefully. This as the somewhat demanding, yet small, initial DFT calculations only need to be carried out once, whereafter the quickly generated COSMO-files can be shared and re-used by the battery R&D community. Furthermore, as the model is totally free of any electrode chemistry/physics, it is totally transferrable between battery designs and with the exception of the need for explicit solvation also between electrolyte solvent composition and concentrations. Indeed, the simplicity and speed are rather remarkable considering that the computational approach uses merely local interactions to predict a macroscopically rather complex property. The successes are perhaps limited at first glance, but the use of more well studied and quality assured experimental solubilities for aqueous systems as a proxy seem to hold some promise.

For future studies, using a much larger set of simple monovalent salts and/or avoiding the three classes of problematic cases above could/would/should most likely improve the overall experimental *vs.* computed solubility agreement. However, our target is rather a general modelling route. But admittedly it is not easy to foresee how to further improve the present model for the intrinsically problematic cases. However, by *e.g.* moving from targeting solely inorganic salts to also include organic SEI species would intrinsically mean less focus on hard as well as divalent cations/anions – and thus be highly beneficial for the COSMO-RS step of the modelling, while again the DFT step might be more demanding, and experimental data be even more scarce (and even less reliable?). Finally, with or even without more experimental data to further refine the model against, we do anyhow believe that the presented strategy can assist in the design of more stable SEIs – not the least needed for battery technologies beyond LIBs.

CRediT authorship contribution statement

Johanna Timhagen: Writing – review & editing, Visualization, Investigation, Formal analysis. **Vigneshwaran Thangavel:** Writing – original draft, Methodology, Formal analysis, Data curation. **Juan Forero-Saboya:** Investigation. **Jonathan Weidow:** Supervision. **Patrik Johansson:** Writing – review & editing, Supervision, Resources, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.electacta.2025.147051.

Data availability

Data will be made available on request.

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