HELIS High energy lithium sulphur cells and batteries

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Title:

D6.1 Databases on electrolyte modelling

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1 SUMMARY

The purpose of this deliverable is to outline the results of the efforts made to collect the modelling files created in WP6 in a database fashion with respect to both direct output files as well as analysis files of molecular level interactions.

2 INTRODUCTION

The electrolytes suggested for HELiS are partly based on studies of interactions, both experimentally and by modelling, between ions, solvents and polysulfides, and how these in turn affect the observed conductivity, viscosity, solubility, etc, and in the end the Li-S cell performance. The modelling efforts in WP6 thus partly targets these interactions. In addition, modelling is made to describe transport and how a continuum description can be used to understand the electrolyte inside the porous cathodes.
The main purpose of D6.1 is to show how we have collected data from Task 6.1 on molecular level interactions for further usage in other tasks within WP6. Furthermore, to provide how the equations used for the continuum modelling have been collected (from Tasks 6.2 and 6.3).
All data collected and created are being made available and searchable.

3 DATABASE NEEDS AND OPTIONS

When revising the possibilities to directly store the output files, prior to any analysis, we must first balance the needs, including the effort in time and space needed, versus the options provided. Here we have looked at several option such as fully fledged systems such as *pymatgen* (which is the Python package behind the Materials Virtual Lab). Pymatgen has a Gaussian support, but however cannot support Turbomole (both these large packages are being used in HELiS). We also looked into options of creating a simple system from combining *CCLib* (a log file parser for comp. chem. programs) and a simple database. For the files arising from the analysis stages and the equations used – the needs are quite different and simpler. Here the main effort has been to construct the format of Excel-sheets to both be user-friendly from an input point-of-view – i.e. the creator of the modelling data and the analysis – and an output point-of-view – i.e. to be understandable for the non-specialist at some reasonable level.

3.1 Output files: Gaussian, Turbomole, COSMO and other files

As already outlined above, we looked at several different options on how to best collect the output files used for the subsequent analysis of the interactions within the electrolytes. The post-processing is very different – for Gaussian and Turbomole the output is most often simple log-files wherefrom a single (or a few) energy data are needed to be extracted, while for in stark contrast COSMO the output can be a direct description of preferred interaction sites between different species – including ion-solvent systems. Given this disparity and to avoid unnecessary overhead to the project, we finally decided for a simple local repository solution where we collect the output files in a catalogue system of Task (can be several)/Topic/extra and a naming system describing the species (or system) and parameters such as method, basis set, etc. One advantage is that the different software names their (sometimes several) output files very differently by the suffixes – and thus we do not need to separately specify the software in the repository.

One example of this database structure:

- Catalogue: 6.1/4.2/fluorination/FDEE/
- File name: FDEE_S4_M06_6311G_CPCM_1_SECIL.log

The above is thus from the Catalogue a calculation made within Task 6.1 (Electrolyte modelling) and coupled to Task 4.2 (Influence of chemical and physical properties) and targeting the role of fluorinated electrolyte solvents via using FDEE (as solvent).

The File name describes that it is the output of a Gaussian09 calculation (the .log suffix provides this information) on a system of a FDEE solvent molecule _and_ an S_4^{2-} polysulfide interacting using the DFT functional M06 and the basis set 6-311G*. It also has made use of an implicit solvent model (CPCM) and is the first generated configuration (1) from the engine software used to create starting guesses (SECIL).

The repository is thus searchable in several ways based merely on a smart and strict naming of files and proper sorting into catalogues. A problem is that over time the optimal Catalogue structure would not be the same as when the repository it was initiated, but this can in worst case by solved by duplication the files to several Catalogues by simple pointers (i.e. no physical copies). We are still working on how to create access to this repository from outside Chalmers (currently not possible due to security restrictions). The disks where the data resides are continuously being subject to back-up so there is minimal risk of data loss. A future action is to also include the FP7/EUROLIS data into the repository.

3.2 Analysis data files

The analysis data files could be created by e.g. semi-automated script-searching the different output-files or by manual extraction of the relevant data after completed calculations. We have here chosen the latter for simplicity, but rather focused on creating Excel-sheets where the interactions (and other outcomes) can be viewed both qualitatively and quantitatively.

From the Gaussian and Turbomole output-files typically one (or more) energies are extracted as pure text and put into Excel-sheets for processing. See below for a straight-forward example of this process and the resulting DEint for two specific solvent-polysulfide interactions.

Input																		Output
Task1	Task2	Target	Solvent1	N1	Solvent2	N2	Solvent3	N3	Cation1	C1	Cation2	C2	Anion1	A1	Anion2	A2	Filenam	Comment	DEint [kJmol-1]
6.1	4.2	Gen1	DIOX	1									S2_2-	1			DIOX_B3	Solv-PS	-66
																	S2_B3LYP_6311G		
6.1	4.2	Gen1	DIOX	1									S4_2-	1			DIOX_B3	Solv-PS	-68
																	S4_B3LYP_6311G		

From the COSMO calculations, the interaction strength and mode is an integrated part of the output and can directly be visualized – but here separate values of interactions are rather input (from Gaussian or Turbomole) than output.

From the mesoporous modelling the outcome is a mix of numerical data and the equations used. The latter are the result of the development of the framework within Tasks 4.2 and 4.3 and are saved within the commented code developed.

4 CONCLUSIONS

A collection of the results from the electrolyte modelling efforts has been made in a repository. Some output has been post-processed in Excel-sheets in order to obtain the interactions within the electrolytes for further comparisons vs. experimental efforts. The structure created is simple and general, to accommodate also future calculations and directions, and searchable, to enable also the non-specialist to use the databases.