How does Lithium-Ion Battery undergo thermal runaway?

A Computational approach to reveal details of battery breakdown process

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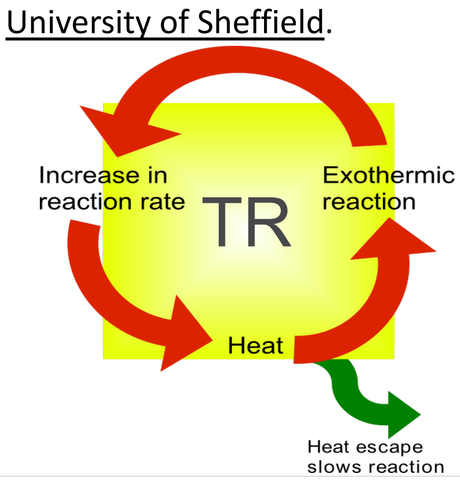
Abstract

Lithium-Ion Battery(**LIB**)often triggers severe disasters as it is highly explosive under extreme conditions. This catastrophic behavior is primarily attributed to LIB thermal runaway(**TR**)which is a positive feedback system causing both temperature and reaction rates to rapidly increase inside LIBs. Therefore, it is of great essence to investigate mechanism of TR to tackle safety issues. The process can be simulated computationally only if chemical Reaction Networks(**RN**) inside LIB is fully understood. Although LIB's RN was worked out previously, its thermodynamic properties and energy profiles haven't been academically studied yet. This poster will demonstrate my studies on RN during my two-month internship.

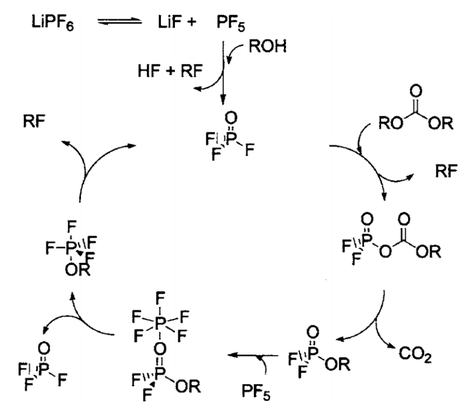
Internship Information

My internship is integrated into an ongoing work of investigating TR mechanism in LIB, which is led by Dr. Peter J. Bugryniec in Prof. Solomon Brown's group in Chemical and Biological Engineering Department at University of Sheffield.



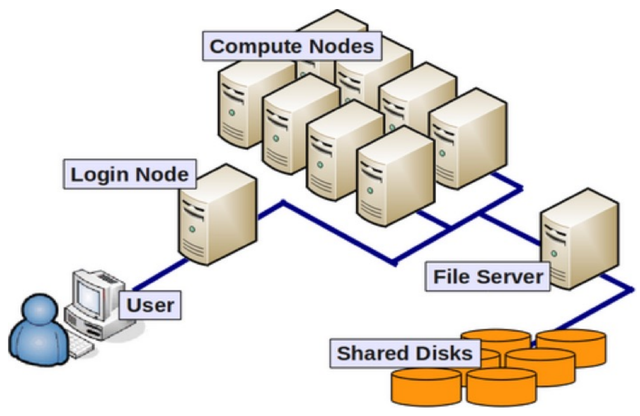
Reaction Network

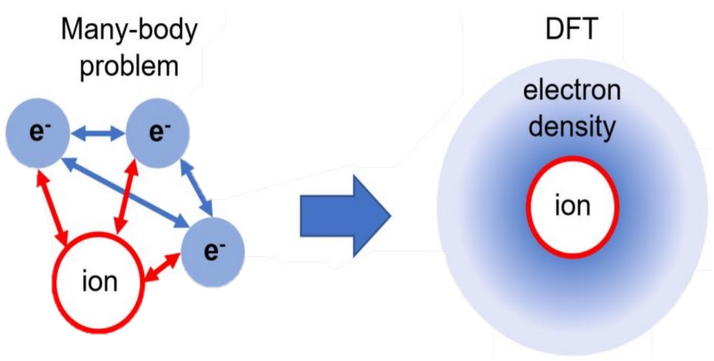
An experimentally deduced RN(Christopher L. Campion *et al* 2005) is adopted. The RN depicts several reactions with presence of Lithium Hexafluorophosphate(**$LiPF_6$**) and Dimethyl Carbonate(**DMC**). They are widely used as salt and electrolyte in LIB, respectively.



Methods

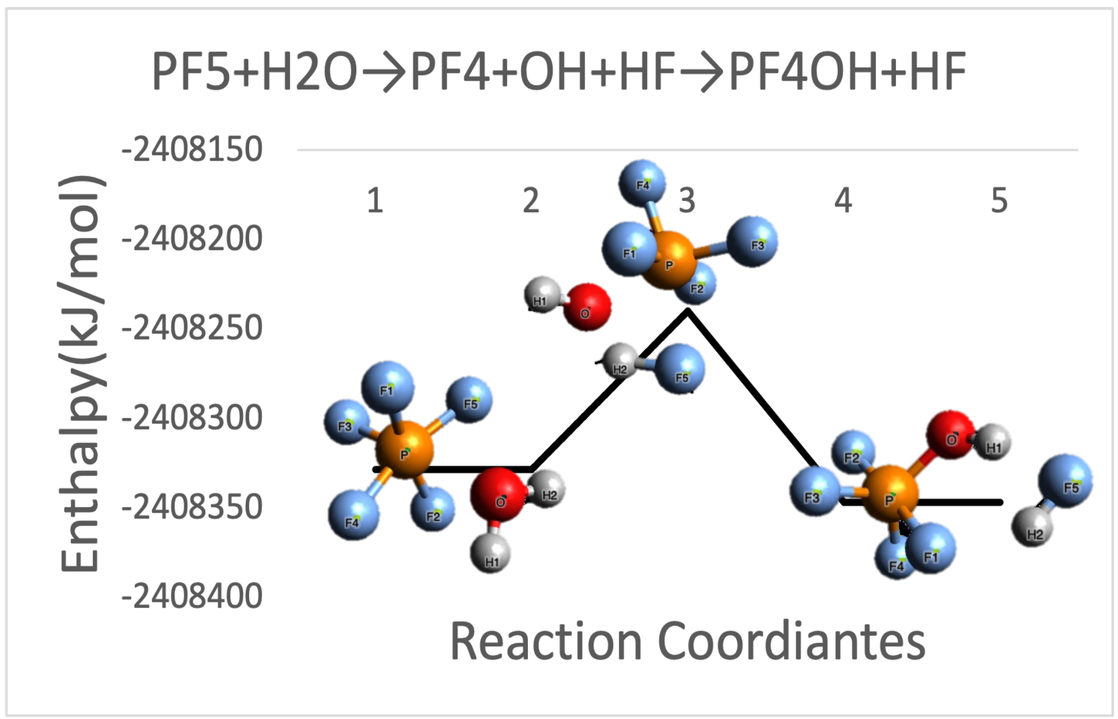
- From the established RN, 7 reactions are generalized.
- Thermodynamic data related to these reactions are gathered. Two software, Gaussian and Avogadro, are crucial to my research.
- Avogadro: This software can be implemented on personal computer(PC), which can visualize molecules. The coordinates of each atom of molecules are recorded and ready to be used as input of Gaussian to do thermodynamic calculations.
- Gaussian: A chemistry software can be run on high-performance computer clusters(**HPC**). It applies density functional theory(**DFC**) to energetically optimize molecules generated by Avogadro. Their thermochemical data are also calculated by Gaussian. Assisted by this method, all reactants, transition states and products in RN can be analyzed thermodynamically and therefore, a full picture of reaction profiles can be generated.





Results

- 7 individual reactions generalized from RN are analyzed.
- Optimized molecules are visualized and their thermodynamic data are calculated and recorded. With these data, reaction profiles are plotted in terms of enthalpies.
- Below shows my analysis of one of the reactions as an example.



Next steps

- My thermochemical data of RN related to $LiPF_6$ and DMC will be combined with previously worked Ethylene Carbonate(**EC**, an electrolyte often co-exists with DMC and $LiPF_6$ in LIB) RN thermochemical data to create a full picture of reactions occurring inside LIBs.
- With these detailed reactions, TR simulation can then be carried out so that behavior of LIB under severe conditions is able to be analyzed.

References

Paper on EC RN:

- Bugryniec, P. J., Yeardley, A., Jain, A., Price, N., Vernuccio, S., & Brown, S. F. (2022). Gaussian-Process based inference of electrolyte decomposition reaction networks in Li-ion battery failure. In Computer Aided Chemical Engineering (Vol. 51, pp. 157-162). Elsevier.

Paper on LiPF6 and DMC RN:

- Campion, C. L., Li, W., & Lucht, B. L. (2005). Thermal decomposition of LiPF6-based electrolytes for lithium-ion batteries. *Journal of The Electrochemical Society*, *152*(12), A2327

ABOUT ME

I am Yuchen Zhao.
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I have a huge interest in battery sciences and I am very passionate with battery safety research.

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