

Cation–Solvent, Cation–Anion, and Solvent–Solvent Interactions with Electrolyte Solvation in Lithium batteries



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The front cover artwork is provided by the group of Prof. Zhang from the department of chemical engineering, Tsinghua University. The image shows the cation–solvent, cation–anion, and solvent–solvent interactions in the electrolytes of lithium batteries, which are similar to the scene of ballet. With electrolyte solvation, these interactions are much weakened, exhibiting longer Li–O/N bond length. Read the full text of the article at 10.1002/batt.201800118.

What was the inspiration for this cover design?

The ballet of Swan Lake.

What prompted you to investigate this topic/problem?

This work is inspired by a question raised by prof. Zhang during a group meeting: Why are the interactions between ions much weaker in solutions than in crystals? The answer based on classical theory is obvious. While first-principles calculations can provide more details for this question at the atomic level, and indeed, some interesting results were obtained.

What is the most significant result of this study?

The cation–solvent, cation–anion, and solvent–solvent interactions in the electrolytes of lithium batteries were comprehensively investigated. With electrolyte solvation, these interactions are much weakened, exhibiting longer Li–O/N bond length. Based on these theoretical results, lithium nitrate was predicted to be dissolved in 1,2-dimethoxyethane (DME) and ethylene carbonate (EC) solvents, which was further validated by experiments. The former was previously widely recognized. However, the latter, the dissolution of lithium nitrate in EC-based electrolyte, is very difficult and arises great interest recently.

Is there any related work in your group recently?

Recently, parts of our work focus on the electrolyte solvation in batteries. Fundamentally, we proposed the concept of ion-

solvent complexes (X. Chen, X. Shen, B. Li, H.-J. Peng, X.-B. Cheng, B.-Q. Li, X.-Q. Zhang, J.-Q. Huang, Q. Zhang, *Angew. Chem. Int. Ed.* **2018**, *57*, 734–737) and unveiled the origin of their reduced reductive stability on metal anodes (X. Chen, H.-R. Li, X. Shen, Q. Zhang, *Angew. Chem. Int. Ed.* **2018**, *57*, 16643–16647). Electrolyte additives, such as fluoroethylene carbonate and lithium nitrate, were thus introduced to regulate the solvation structure of Li-ions in electrolytes (X.-Q. Zhang, X. Chen, X.-B. Cheng, B.-Q. Li, X. Shen, C. Yan, J.-Q. Huang, Q. Zhang, *Angew. Chem. Int. Ed.* **2018**, *57*, 5301–5305; X.-Q. Zhang, X.-B. Cheng, X. Chen, C. Yan, Q. Zhang, *Adv. Funct. Mater.* **2017**, *27*, 1605989). With optimized electrolytes and thus a stable solid-electrolyte interphase formed, desirable electrochemical performances of both coin and pouch cells were achieved (X. Chen, T.-Z. Hou, B. Li, C. Yan, L. Zhu, C. Guan, X.-B. Cheng, H.-J. Peng, J.-Q. Huang, Q. Zhang, *Energy Storage Mater.* **2017**, *8*, 194–201; C. Yan, X.-B. Cheng, Y. Tian, X. Chen, X.-Q. Zhang, W.-J. Li, J.-Q. Huang, Q. Zhang, *Adv. Mater.* **2018**, *30*, 1707629; X.-Q. Zhang, X. Chen, R. Xu, X.-B. Cheng, H.-J. Peng, R. Zhang, J.-Q. Huang, Q. Zhang, *Angew. Chem. Int. Ed.* **2017**, *56*, 14207–14211).

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