Topics in Current Chemistry Collections

Aims and Scope

The series *Topics in Current Chemistry Collections* presents critical reviews from the journal *Topics in Current Chemistry* organized in topical volumes. The scope of coverage is all areas of chemical science including the interfaces with related disciplines such as biology, medicine and materials science.

The goal of each thematic volume is to give the non-specialist reader, whether in academia or industry, a comprehensive insight into an area where new research is emerging which is of interest to a larger scientific audience.

Each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole. The most significant developments of the last 5 to 10 years are presented using selected examples to illustrate the principles discussed. The coverage is not intended to be an exhaustive summary of the field or include large quantities of data, but should rather be conceptual, concentrating on the methodological thinking that will allow the non-specialist reader to understand the information presented.

Contributions also offer an outlook on potential future developments in the field.

More information about this series at http://www.springer.com/series/14181

Martin Korth
Editor

Modeling Electrochemical Energy Storage at the Atomic Scale

With contributions from

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Preface

It has become apparent that electrochemical energy storage is going to play a central role for our energy future. Current storage devices are unfortunately not yet as safe, cheap and efficient as we would need them to be for a quick exit from fossil fuels. Fortunately, tremendous efforts are made both experimentally and more recently also theoretically to understand the above mentioned problems in detail and to work on economically viable solutions or alternatives. The challenges cannot be overlooked, especially on the theoretical side. While more and more substances are coming into consideration as possible electrode or electrolyte materials, knowledge about the basic storage processes is still very limited. The complexity of real materials is causing great problems here, but also the fact that there is no generally applicable, black-box computational model available to treat physical systems at the atomic scale under electrochemical conditions, i.e., including the effect of electrolytes and electrode potentials. It has nevertheless become clear that such methods and the knowledge we could gain from them are key for innovating electrochemical energy storage, as any rational design of essentially redox-based devices will require a quantum-mechanical understanding of atomic-scale structures and reactivity.

With this publication, we present studies from five research teams who dare to venture into the unknown of electrochemical energy storage at the atomic scale.

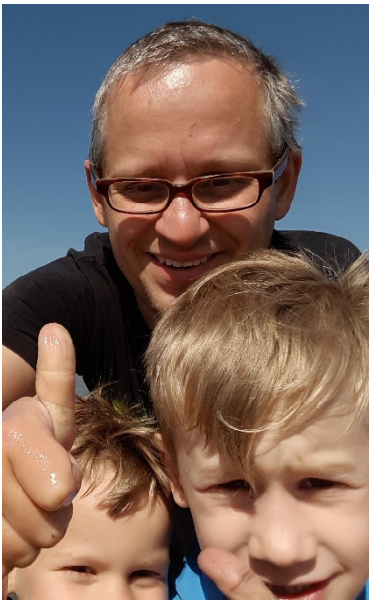
We start with Groß, who discusses the technical obstacles we face when applying computational methods and especially those from quantum chemistry to electrochemical energy storage systems.

The second contribution gives the complementary view from a leading experimental group with a focus on current battery technology and a discussion of where help from modeling and simulation would be most welcome.

Rempe and co-workers then give us a classical mechanics view of electrolytes, before Rajput *et al.* Persson review the current state of investigations into complex (here multivalent) electrolytes, where theory can at least help to understand and organize contradictory experimental results.

We finish with Viswanathan and co-workers, who show us how to build a bridge from theory to experiment with the development of design principles for new device types (here Lithium-Oxygen batteries), keeping both electrodes and electrolyte features in mind.

We hope that the presented contributions inspire more theoreticians to turn at least part-time to theoretical electrochemistry, not only because of the great importance it has for societies around the globe, but also for the intellectual challenges it poses and last but not least for the fun of it. We also hope to have convinced one or the other experimentalist of the value of atomic-scale theoretical investigations into electrochemical experiments. For having made this a possibility, we would like to thank all authors for their valuable contributions.



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