"Next generation computational tools for the design and optimization of the next-generation electrochemical energy devices"

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Thanks to the development of the modern computational science over the past few decades, multiscale modeling and numerical simulation are emerging as powerful tools for *in silico* studies of mechanisms and processes in electrochemical cells for energy storage and conversion such as secondary batteries. These innovative approaches allow linking the chemical/microstructural properties of materials and components with their macroscopic efficiency and deserve as powerful tools for the analysis of experimental data. Moreover, upon appropriate experimental validation, they can potentially provide tremendous progress in designing and optimizing the next-generation cells.

In this seminar I will present a comprehensive overview of the fundamentals and practical aspects of some of the multiscale modeling activities ongoing in our laboratory within the context of electrochemical energy R&D. Several application examples will be provided, including on next-generation lithium ion, lithium air, lithium sulfur and redox flow batteries, fuel cells and dye-synthesized solar cells. Finally, I will discuss technical dreams and methodological challenges being faced today towards the development of the next-generation computational tools in academia and in industry.

References

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