An introduction to the atomistic design of materials for electrochemical energy storage

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The symposium is introduced with an overview on the state-of-the-art of electrochemical energy storage and how computational materials science accelerates the screening of new materials enabling alternative low-cost storage systems.

In recent years research is focusing on the discovery of new materials enabling alternative low-cost storage systems according to the fact that 50% to 70% of the battery total cost is accounted by by components' materials.

Materials science has been greatly affected by the advancements in HPC and Big Data technologies, and a new kind of dynamics between theory and experiment is in progress. The different atomistic approaches adopted to design anode, cathode and electrolyte, and some examples of automation, advanced analysis and predictive capabilities are outlined.