Powering Next-Gen Batteries-using multi-scale simulation

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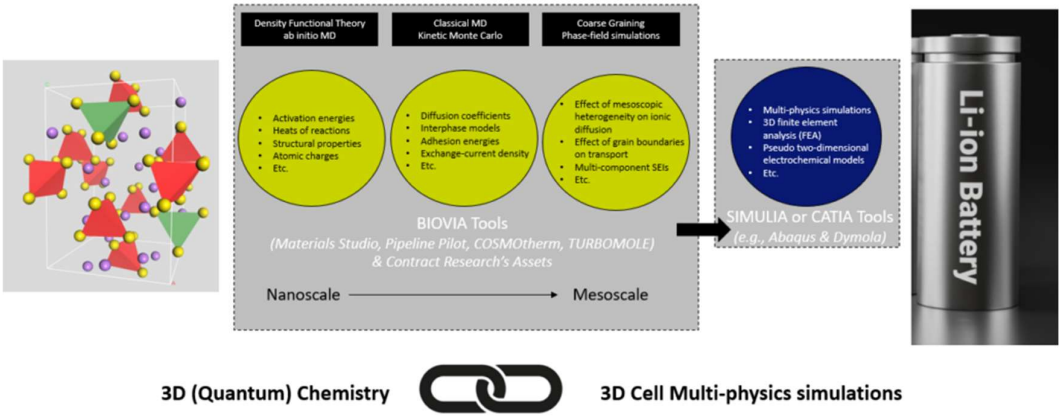
In today's world, the demand for clean, efficient, and sustainable energy is growing rapidly. The development of next generation batteries is crucial to meet this demand and reduce our reliance on fossil fuels. However, creating these innovative batteries is no easy task. It requires cutting-edge research, development, and testing of advanced materials that can enhance battery performance, durability, and safety. On the other hand, batteries are extremely complex devices; to just name a few of such complexities: a variety of materials with various (electrical and mechanical) properties and topologies form at the electrochemical interface between the anode/cathode and the electrolyte. Also, the electrolytes themselves are often a soup of different components. Therefore, to simulate such a battery, one cannot afford to use quantum chemical atomistic modeling to calculate the most important electrical or thermal properties of the system: it is unimaginably computationally taxing. That is what necessitates the multiscale simulations. The example multi-scale scenario covering the nanoscale to macroscale workflow is shown in the figure below [1]:



In thjis talk examples on multi-scale simulation, to deliver multiscale workflow for different components of battery electrode, electrolyte [2] and SEI [3] to deisgn and analyse the complicated battery design..

References

1. https://blog.3ds.com/brands/biovia/bridging-the-gap-between-quantum-mechanics-battery-cell-design/
2. Hanke, F, *et al* 2020 *J. Electrochem. Soc.* **167** 013522
3. Abbott, J.W,; Hanke, F.. ChemRxiv. 2021; 10.33774/chemrxiv-2021-l8c7b