To address the future energy demands, it is essential to develop scalable energy storage systems from abundant materials that can be integrated with renewable energy. For centuries, batteries have been known for their excellent chemical energy conversion and storage. Most portable energy storage technology is currently dominated by lithium-ion while stationary energy storage with lead acid-based technology. The intercalation-based lithium-ion technology has high energy density but is still expensive to scale up. Less abundance of lithium and the safety due to the use of liquid organic electrolytes are primary concerns. While on the other hand, conversion reaction-based lead acid batteries cause significant environmental problems with low energy density and limited cycle life require exploring an alternate energy storage technology.

The current state of the art for lithium-based technology has a positive electrode of \( \text{LiCoO}_2 \) or its derivatives or spinel compound like \( \text{LiMn}_2\text{O}_4 \) or polyanionic compound like \( \text{LiFePO}_4 \). The present research can be divided into two categories: the first one focuses on the cost and safety with the expense of energy density, while the other is to improve the energy density, whereas the demand for optimum performance lies in both. Recently, partial replacement of transition metal sites with the lithium known as lithium-rich compound showed very high capacity ~300 mAh/g but suffered from a poor cycle life [1]. Apart from lithium, other cations like K+, Na+, Zn+2, Mg+2, Al+3, etc. have been explored for energy storage. However, none were found suitable. Similar mono-valent Na and K-based ions show poor cycle life due to the bigger size of the intercalating ions. The multivalent ions, though they have an ion size close to the Li+ but high electric density due to greater charge, will result in strong electrostatic interaction with the host material, resulting in a polarization effect that sluggish the diffusion process.

The search for better technology for the future based on earth-abundant materials like Na+ and Zn+2 requires much scientific exploration to make these technologies feasible on the device level. As seawater is an infinite source of sodium elements and is an abundant material. The concentration of Na+ ions in seawater is approximately 0.47 M. It can possibly act as a Na+ ion source during the direct use of sea water in batteries. But the suitable electrode material requires more scientific examination for the commercialization of these technologies. Similarly, India lies in 7th place in terms of zinc reservoirs and 3rd place in the production of the world’s 5.3% zinc, which attracts researchers for zinc-based technology. Zinc metal has a theoretical specific capacity of 820 mAh/g. A capacity density of more than two times that of lithium, equal to 5855 mAh/cm³ makes it a potential material for energy storage application and needs to be explored [2].

With the advancement of computer’s power will help design and analyze experiments via computations to better understand the underlying physicochemical factors, which will result in the development of next-generation energy storage devices, electrode materials and solid and liquid electrolytes. The rate of charging and discharging, stability, and overall efficiency of any battery is highly dependent on the structural and transport properties of the electrolytes. The atomistic and molecular level simulations would help understand the ion hopping (Li+, Na+, Mg+2, Zn+2, and Al+3, etc.), ion dynamics, ionic conductivity, transference number, and solvation thermodynamic properties in different electrolytes and electrode materials. On the other hand, it is known that solvated ions in the liquid electrolytes influence the overall reaction rate and selectivity. Thus, fundamental gaps such as accurate understanding of the reaction kinetics in different electrolyte materials and their effects due to different perturbations are challenging, which need to be understood in more detail. A combination of atomic-level simulations such as Density Functional Theory (DFT), Molecular dynamics (MD) simulations, and Coarse-grained (CG) simulations along with the experimental benchmarks, will help in developing the next-generation batteries. Figure 1 presents research directions towards the combined computational and experimental approach toward this multi-dimensional battery material development problem.
Further, to enhance the battery performance, different electrolytes are being considered such as water-in-salt electrolytes [3], polymer electrolytes [4], etc. However, there are challenges such as developing enhanced sampling techniques for the electrochemical reactions in the solid-liquid interfaces, implementing Machine Learning (ML) approaches to understand the physicochemical properties of liquid electrolytes [5], and estimating the lifetime of both electrolyte and electrode materials. Considering modern computing resources such as GPUs and web-based cloud technologies, this combination of approaches would enable the researchers to solve this complex problem.

References:


About the Authors