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Sogang CBE Online Talk Series

Accelerating Materials Design and Discovery via High-Performance Computing

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The discovery and design of new materials has long played a key role in enabling technological advances across a wide range of industries. Especially for low-cost clean energy technologies to be economically competitive with fossil fuels, we need to develop new energy conversion and storage materials that are cheaper, more efficient, more abundant, and safer than those currently used. We should also make the materials discovery, development, and deployment faster, less expensive, and more predictable. Experiment can provide many clues to the behavior of candidate materials, but the interpretation is often controversial due largely to the difficulty of direct characterization. Under such circumstances, first-principles computational approach has emerged as a powerful alternative for the understanding and optimization of complex materials and processes. After a brief introduction to first-principles modeling of materials, this talk will focus on discussing materials challenges in rechargeable batteries and the role of computation in overcoming them. Lithium ion batteries (LIBs) are currently widely used in portable electronic devices and electric vehicles (EVs). However, in order to extend their effective use as large-scale energy storage systems for next-generation EVs and renewable energy, there is an imminent need to further increase the energy density, power density, and cycle life while retaining safety and cost at an affordable range. In addition, all-solid-state lithium-metal batteries (ASSLMBs) have recently garnered considerable attention due to their advantages in terms of energy storage capacity and safety over LIBs. However, the large interfacial impedance originating from poor physical contact and/or parasitic reactions at the electrode/electrolyte interface hinders the development of ASSLMs. The challenge involves developing a firm understanding of electrode and electrolyte materials as well as the structure and chemistry at their interfaces, which has been greatly assisted by systematic computational investigations.

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