Atomistic Modeling and Artificial Intelligence for Materials Discovery

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The discovery and development of the novel material take an average of 18 years to commercialize and requires the huge amount of manpower and resources [1]. The Edison-type trial-and-error method has limitations in the development of high-performance materials especially in the field of energy. First-principles calculations can provide in-depth understanding on the reaction mechanisms that can guide designing new materials [2,3]. High-throughput screening with first-principles calculation allow us to explore large materials space efficiently [4]. Also, it is expected that self-driving laboratories with artificial intelligence and robotics can accelerate the development of new materials. In this talk, I will present the first-principles results on the electrode materials for Li-ion batteries [2,3] and the mixed ionic and electronic conductors for solid-state Li-air batteries [4]. I will also briefly introduce our recent progress on the self-driving laboratories to discover new materials for Li-ion batteries.

[1] *Nature Mater.*, 12, 173 (2013)

[2] *Nature Chem.*, 8, 692 (2016)

[3] *Science*, 367 (6481) 1030 (2020)

[4] *Adv. Energy Mater.,* 10(38) 2001767 (2020)