A Priori Search of New Battery Physics

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Abstract

Richard P. Feynman first suggested the possibility of simulating physics on computers and what it entails[1]. Since then, approximations of the underlying physical laws and their mapping to numerical algorithms have been developed. This representation of quantum mechanics allows seeing the physical world of systems first in theory and then the experimental reality follows. The subject of debate is the order of their occurrence. Here, we present state-of-the-art methods derived from this philosophy, capable of uncovering new physics in the realm of material science. Further, from a broader context, the scope of this work is aimed at discovering new phenomena in materials of interest, particularly to the industrialists in the energy storage sector. The importance of ab initio methods in materials physics is illustrated and recent evidence from our recent work is put forth.

As we make progress as a civilization, it incurs a cost associated with increased energy consumption, resulting in a surge of carbon emissions. This calls for the development of clean energy production and storage strategies[2]. The energy storage industry has witnessed a revolution since the onset of Lithium-Ion and Batteries (LIBs). Owing to the versatility in a multitude of applications, LIBs have become a forerunner when it comes to storing energy for the operation of portable electronics and automobiles. Researchers have showcased different classes of materials successfully as candidates at a commercial scale. Here a historical account of an important family of spinel materials is presented. Spinel materials are crucial to the modern-day energy storage industry, particularly for the intercalation battery framework. One of the most promising compositions for battery cathodes are oxides of Manganese-earth abundant, nontoxic, yet economically viable candidates. Manganese-based materials are promising Cobalt-free alternatives, sourcing the latter being acclaimed as giving rise to human ethics violations. However, the manganese oxide spinel suffers from degradation mechanisms occurring during battery cycling[3]. To date, experimental shortcomings due to instrumental resolution have failed to shed light on the causal phenomenon of the degradation processes. We present computational methods enabling physics-guided searches in a wide variety of processes associated with energy storage and conversion applications[4].

References

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