Harnessing Machine Learning for Advancing Amorphous Battery Materials

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Many materials with applications in energy, e.g., batteries, are non-crystalline or exhibit complex chemical disorder and multicomponent compositions. This complexity makes direct modeling with first-principles methods challenging. To address this challenge, we developed accelerated sampling strategies based on machine learning interatomic potentials (MLIPs), genetic algorithms, and molecular dynamics simulations [1]. Here, I will discuss the methodology and its applications to both amorphous and crystalline battery materials. For amorphous materials, we constructed the phase diagram of LiSi alloys, which are prospective anode materials for lithium-ion batteries [2], and mapped the composition-structure space of lithium thiophosphate (*LiPS*) solid electrolytes [3-5], correlating thermodynamic stability and ionic conductivity with local structural motifs to identify structure-composition-property relationships. For crystalline layered oxides, our recent work demonstrates the use of MLIPs for direct atomistic simulations of LiNi0.8Mn0.1Co0.1O2 (*NMC811*), enabling efficient and accurate prediction of Li-ion transport properties that would be computationally prohibitive with conventional first-principles methods.

Complementing these simulations, X-ray absorption spectroscopy (XAS) provides local chemical insights; we established an S/P/O K-edge XAS databases for *LiPS* / *NMC811* materials using simulated structures [3]. Together, these studies illustrate how ML-driven simulations integrated with spectroscopic analysis can accelerate the understanding and design of complex battery materials at the atomic scale.

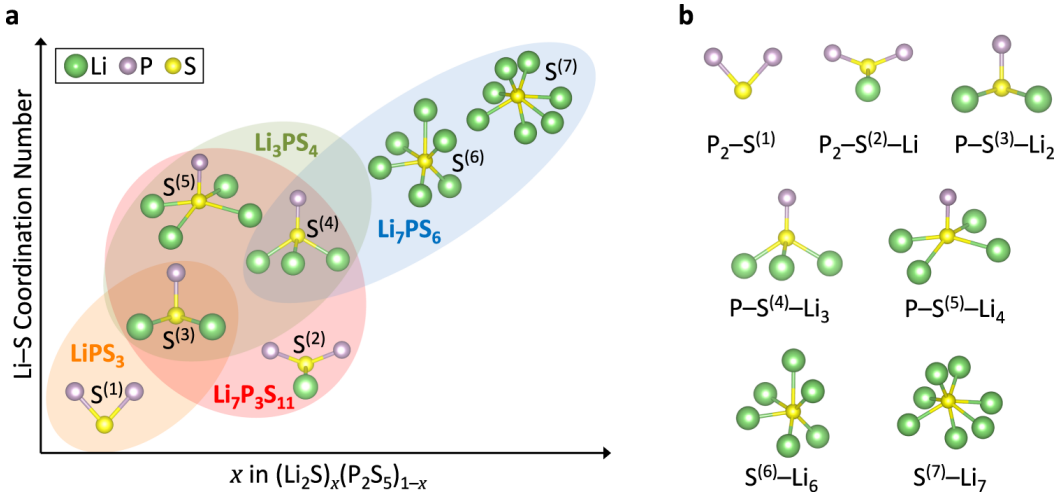

Figure 1: Schematic illustration [4] of the local coordination of S atoms with Li and P atoms in selected $(Li_2S)_x(P_2S_5)_{1-x}$ crystalline structures. Li: green; S: yellow; P: purple. $LiPS_3$: orange region; $Li_7P_3S_{11}$: red region; Li_3PS_4: green region; Li_7PS_6: blue region.

References:

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