Understanding the Structure of Amorphous Na–P Battery Anodes with Machine Learning

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Elemental phosphorus has emerged as a promising anode material for sodium-ion batteries, offering a high theoretical capacity of 2596 $mAhg^{-1}$ in its fully sodiated Na_3P phase [1]. Among its allotropes, black P and amorphous red P have been extensively studied, often in composite form with conductive carbon materials to enhance cycling stability [2]. Notably, amorphous Na–P phases are commonly observed as intermediates during cycling, yet their structural evolution and role in sodium storage remain poorly understood.

The Zintl–Klemm concept has long been used to explain and predict the bonding and structures of crystalline solid-state materials [3]. In this work, using first-principles simulations combined with state-of-the-art machine-learning (ML) methods, we provide atomic-scale insight into the structural and energetic behaviour of amorphous Na–P phases. Our simulations are based on the MACE architecture for fitting message-passing ML interatomic potentials [4]. Subsequent analyses reveal the applicability of Zintl–Klemm rules in the amorphous state.

References

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