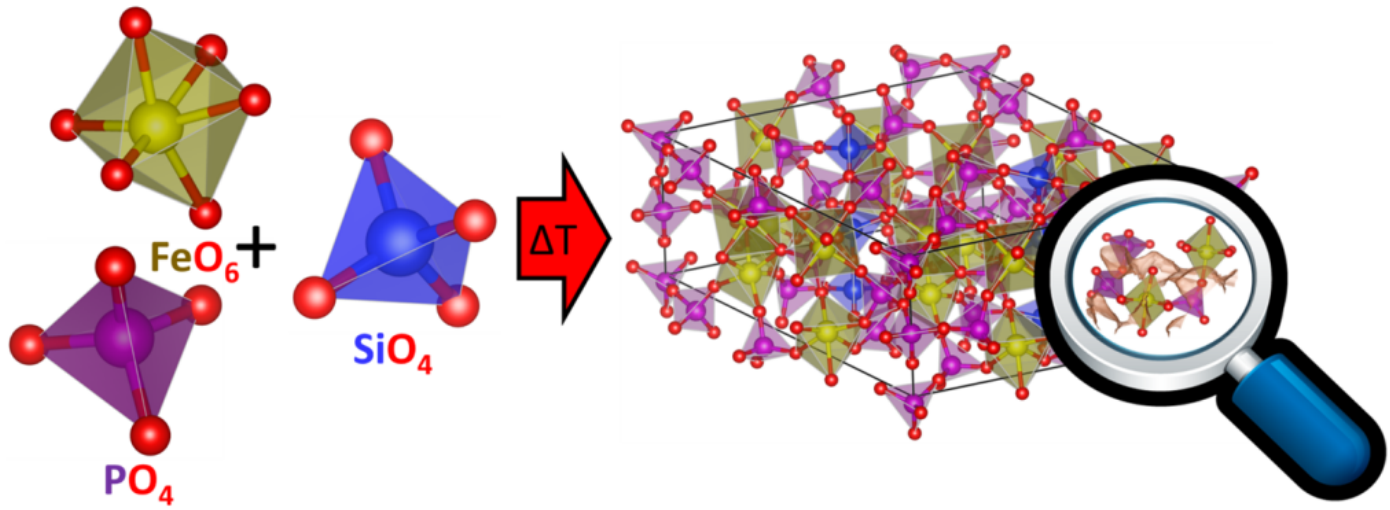
The First Fe-based sodium-ion cathode with two distinct type of polyanions

The current lithium-ion battery technology finds wide applications, powering cell phones, laptops, and electric vehicles. In 1991, Sony announced the first-generation of commercial Li-ion batteries, which composed of $LiCoO_2$ cathode and graphite anode. Such cells have the drawback of safety concerns due to the liberation of oxygen from $LiCoO_2$ at deep charge. Due to safety concerns, only half of the theoretical capacity of $LiCoO_2$ can be used in practical cells.



To overcome the above difficulties, various alternative cathodes have been explored during the past three decades. Among them, cathodes consisting of poly-anions (XO_4^{n-}; X = S, P, and Si; n ? 2) offer superior thermal stability. An excellent example is $LiFePO_4$, reported in 1997. For most of the polyanion cathodes reported, the structure is composed of only one type of XO_4^{n-} (X = S, P, or Si) groups. Na-ion batteries are attracting much attention recently due to the high abundance and low cost of sodium as an alternative to lithium-ion batteries.

Recent work published in the *Chemical Communications,* by Wang Hay Kan and Arumugam Manthiram at the University of Texas at Austin and Ashfia Huq at the Neutron Scattering Science Division at Oak Ridge National Laboratory, has shown that a Na-ion cathode $Fe_3P_5SiO_{19}$ with two types of XO_4^{n-} (X = P and Si; n ?2) groups exhibit a reversible capacity of ca. 70 mAh g^{-1}, *i.e.,* 1.7 Na^+ ions per formula can be reversibly inserted/extracted at an average voltage of 2.5 V versus Na^+/Na. To understand the Na^+-ion conduction pathway, bond valence sum (BVS) mismatch minimization procedure was performed. The low isovalence surfaces are located around the unfilled interstitial sites around the Fe_2O_9 dimers, phosphates and disilicates. A lower mismatch pathway along z-axis is found, suggesting its anisotropic ionic conductivity.

Overall, this study highlights the importance of cathodes with multiple polyanions and their physical

properties and electrochemical performances.

Publication

The first Fe-based Na(+)-ion cathode with two distinct types of polyanions: Fe3P5SiO19.
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