Magnetic Structure and Properties of $NaFePO_4$ Polymorphs: Antiferromagnetic Ordering and Spin-Flop Transition

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Abstract

In recent years, the cost and sustainability concerns have renewed research efforts on sodium-ion batteries, propelling investigation on various layered oxides and polyanionic family of insertion compounds for low-cost and large-scale cathode applications. These cathode insertion compounds are functional materials, involving redox active 3*d* transition metals (e.g. Fe/Co/Ni) that are often magnetic in nature. During the Na (de)insertion process involving redox reaction of transition metals and structural alteration, the magnetic magnetic structure/ properties can vary significantly.

We have investigated the magnetic structure and properties of $NaFePO_4$ polyanionic system, which exists in two distinct polymorphs: metastable *triphylite* and stable *maricite*. The details of these structures are shown in the figure. Both these polymoprhs undergo antiferromagnetic ordering below 50 K (for *triphylite*) and 13 K (for *maricite*). Using the magnetic susceptibility, heat capacity and low temperature neutron powder diffraction, the magnetic structure of these two distinct polymorphs have been solved. The details of these antiferromagnetic structures will be described considering the

super- and super-superexchange interactions. In addition, investigating the *maricite* $NaFePO_4$ polymorph, which consists of edge-sharing FeO_6 octahedral chains, we have discovered the occurrence of spin-flop transition below 40 kOe using susceptibility measurement and low-temperature Mossbauer spectroscopy. This spin-flopping (or metamagnetism) phenomenon in *maricite* $NaFePO_4$ will be described in detail [1-5] to showcase the rich magnetism present in $NaFePO_4$ insertion materials.

References:

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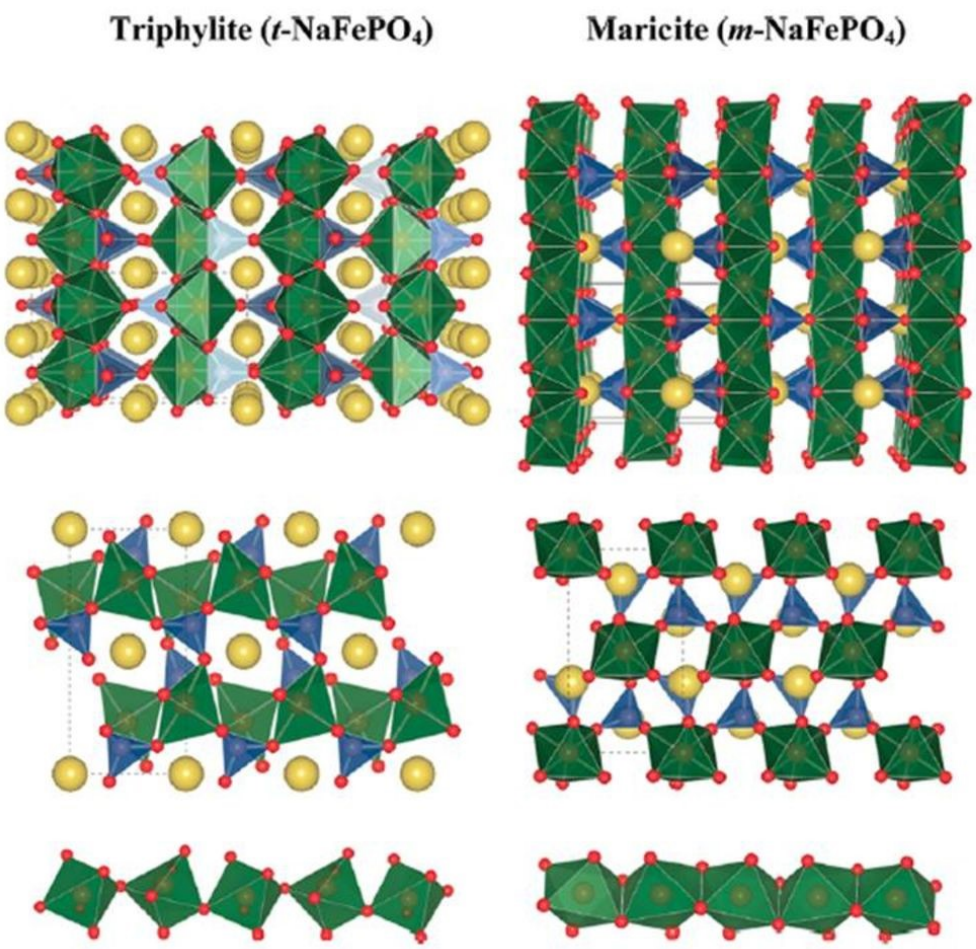

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