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Magnetic Phase Transitions of New Sodium-ion Battery Cathode $\text{Na}_4\text{Ni}_7(\text{PO}_4)_6$

Sodium-ion batteries (NIB) are of intense current interest as alternatives to lithium-ion batteries for large-scale applications in which kinetics and weight are not the primary consideration. However, the jury is still out on the ultimate competitiveness of NIB versus other energy storage solutions, with one major uncertainty being a lack of Na electrode materials. [1] Monoclinic $\text{Na}_4\text{Ni}_7(\text{PO}_4)_6$ has demonstrated a great potential to be a new electrode candidate in our recent study. In addition, its complex magnetic properties also attracted our interest. [2] In this presentation, we mainly focus on investigation of the magnetic phase structures of $\text{Na}_4\text{Ni}_7(\text{PO}_4)_6$. According to the magnetic susceptibility analysis and variable temperature neutron diffraction measurements, $\text{Na}_4\text{Ni}_7(\text{PO}_4)_6$ presents three successive antiferromagnetic (AFM) ordered phases (Phase I, Phase II and Phase III) at 9.1-17K, 4.6-9.1K and <4.6K respectively, with the magnetic ordering vector $[0, 1, 1/2]$, $[0, 2/3, 1/2]$, and $[0.076, 2/3, 1/2]$, refer to the nuclear unit cell. The magnetic ordering shows distinct ferromagnetic (FM) Ni^{2+} strips and antiferromagnetic arrangements between FM strips. The moment amplitude of all strips is equivalent in Phase I but varies in Phase II. Phase III is an incommensurate structure and should have a similar spin arrangement with Phase II.

References

- [1] Hyungsub Kim, *et al.*, Recent progress in electrode materials for sodium-ion batteries, *Advanced Energy Materials* 2016, 6, 1600943.
[2] Qingbo Xia, *et al.*, Magnetic phase transitions and sodium ionic conductivity of $\text{Na}_4\text{Ni}_7(\text{PO}_4)_6$, *Inorganic Chemistry* 2018. (Submitting)

Topic

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