

Abstract Submitted  
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**Phase diagram of Na<sub>1-x</sub>Ca<sub>x</sub>V<sub>2</sub>O<sub>4</sub> compounds synthesized at high pressure** TAMAS VARGA, JOHN MITCHELL, Argonne Natl Lab, KAZUNARI YAMAURA, DAVID MANDRUS, Oak Ridge Natl Lab, JUN WANG, Argonne Natl Lab — Ambient pressure CaV<sub>2</sub>O<sub>4</sub> and high-pressure NaV<sub>2</sub>O<sub>4</sub> crystallize in the CaFe<sub>2</sub>O<sub>4</sub> structure type containing double chains of edge-sharing VO<sub>6</sub> octahedra. Recent measurements on NaV<sub>2</sub>O<sub>4</sub> reveal low-dimensional metallicity and evidence of half-metallic ferromagnetism. In contrast, CaV<sub>2</sub>O<sub>4</sub> is an antiferromagnetic insulator. To explore the evolution of these ground-state behaviors, we have prepared a series of Ca-doped NaV<sub>2</sub>O<sub>4</sub> compounds with the formula Na<sub>1-x</sub>Ca<sub>x</sub>V<sub>2</sub>O<sub>4</sub> (x=0-1) using high-pressure synthesis. The lattice parameters of Na<sub>1-x</sub>Ca<sub>x</sub>V<sub>2</sub>O<sub>4</sub> samples change with nominal x according to Vegard's law. The metallic state in NaV<sub>2</sub>O<sub>4</sub> is dramatically altered by Ca doping. Samples with higher Ca concentrations (x=0.6-0.8) exhibit a metal-insulator transition around 150 K. Samples at the Na end (x=0-0.2) show a broad antiferromagnetic transition in the 120-160 K range in accordance with earlier reports. With increased Ca doping, the antiferromagnetic transition is suppressed to ~70 K at the Ca-endmember. Transport measurements show an insulator-metal transition at x~0.4. Comparison to existing studies at the Ca- and Na-rich ends will be discussed along with a schematic (T-x) phase diagram for the Na<sub>1-x</sub>Ca<sub>x</sub>V<sub>2</sub>O<sub>4</sub>.

Tamas Varga  
Argonne Natl Lab

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