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Interplay between structure and properties in $TlFe_{1.6}Se_2$[1] ANDREW MAY, HUIBO CAO, MICHAEL MCGUIRE, CLAUDIA CANTONI, BRYAN CHAKOUMAKOS, RADU CUSTELCEAN, BRIAN SALES, Oak Ridge National Laboratory — The degree to which Fe vacancies order greatly influences the properties of intercalated FeSe compounds. In this talk, we will consider the relationship between vacancy ordering and the properties of $TlFe_{1.6}Se_2$. Unlike the alkali-metal based compounds, such as $K_{0.8}Fe_{1.6}Se_2$, $TlFe_{1.6}Se_2$ does not become superconducting and always forms with the Tl-sites fully occupied. This results in reduced complexity and disorder, allowing the role of Fe vacancies to be probed directly. Common to all of these materials is $\sqrt{5}a \times \sqrt{5}a$ superstructure associated with ordering of the Fe vacancies, which appears coupled to a block-checkerboard antiferromagnetic order. Through subtle changes in composition and processing, the vacancies can order more or less completely, and this results in substantial variations in the magnetic properties of $TlFe_{1.6}Se_2$. The electronic behavior is relatively insensitive to these changes, though, as semiconducting behavior is observed in all cases. Finally, high resolution TEM reveals complex local structures, which are markedly different from those observed in $K_{0.8}Fe_{1.6}Se_2$.

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