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Selective d-band Participation in Magnetic and Electronic Behavior of Spin-Ladder Iron-chalcogenides JOSEPH CARON, JAMES NEILSON, DAVID MILLER, The Johns Hopkins University, VADIM KSENOFONTOV, CLAUDIA FELSER, Johannes Gutenburg University, KATHRINE ARPINO, The Johns Hopkins University, ANNA LLOBET, Los Alamos National Laboratory, TYREL MCQUEEN, The Johns Hopkins University — The mechanism of superconductivity in the iron-based superconductors, particularly the role of magnetism and band nesting, remains controversial. The iron-based superconductors share many properties with the high-T_c cuprates, including two-dimensional layers and proximity to magnetic order. Using reduced dimensionality, as exemplified by the "spin ladder" cuprates, we attempt to understand the electronic and magnetic behavior of the $A\mathrm{Fe}_2X_3$ (A= alkali or alkali earth, X = chalcogenide) family of materials. These compounds have $2 \times \infty$ double-chains ("ladders") of edge-sharing $\mathrm{Fe}X_4$ tetrahedra, cutouts of the full two-dimensional Fe_2X_2 layers of the iron-based superconductors which provide a platform from which to understand the interplay of structure, magnetism, and electronic behavior. The unique properties of these compounds is exemplified by both the inability of DFT programs recapitulate either the underlying physical properties or the dramatic transition from block to stripe magnetic order in $\mathrm{Ba}_{1-x}\mathrm{K}_x\mathrm{Fe}_2\mathrm{Se}_3$ that coincides with a change from magnetic to non-magnetic behavior of one d- orbital-derived band. I will also present the influence of pressure and chemical doping on metallic and/or superconducting behavior.

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