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Local Displacements, Magnetoelastic Coupling, and Bonding in Spin-Ladder Iron Selenides JAMES NEILSON, JOSEPH CARON, DAVID MILLER, Johns Hopkins University, ANNA LLOBET, Los Alamos National Laboratory, TYREL MCQUEEN, Johns Hopkins University — The spin-ladder "1-2-3" compounds $BaFe_2Se_3$ and KFe_2Se_3, built of double-chains of edge-sharing $[FeSe_4]$ tetrahedra, are localized-moment antiferromagnetic semiconductors. Total neutron scattering of $BaFe_2Se_3$ reveals local iron displacements coupled to long-range ordered antiferromagnetism comprised of ferromagnetic Fe_4 plaquettes. The magnitude of the iron displacements follow the antiferromagnetic order parameter: a manifestation of magnetoelastic coupling. These local displacements are essential for properly understanding the electronic structure of these systems, as local structural modulations necessarily perturb the ground state wavefunctions. Furthermore, while iron displacements from magnetoelastic coupling in FeX_4-based materials are hypothesized to be important in the emergence of superconductivity, the spin-ladders remain insulating down to 1.8 K, even upon hole doping by substitution of K for Ba. As with the copper oxide superconductors two decades ago, our results highlight the importance of reduced dimensionality spin-ladder compounds in the study of the coupling of spin, charge, and atom positions in superconducting materials.

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