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Electronic structure and magnetic excitations in iron selenides MARK VAN SCHILFGAARDE, King's College, London, UK, LIQIN KE, VLADIMIR ANTROPOV, Ames Laboratory — We calculate the electronic structure and magnetic excitations in the $K_4Fe_{4+x}Se_5$ alloy, with x between 0 and 1, within the local-density approximation. Analysis of the electronic structure with varying x leads to a prediction of the coexistence of two phases: one, strongly magnetic and another, weakly or nonmagnetic. Using linear response techniques we calculate spin wave spectra in $K_4Fe_{4+x}Se_5$, and find it is in excellent agreement with a recent experiment. The spectrum can be described rather well by an anisotropic J_1-J_2 model. We confirm that exchange coupling between NN Fe magnetic moments is strongly anisotropic, and show directly that in the ideal system this anisotropy can be associated with higher order terms in spin Hamiltonian (biquadratic coupling). Structural relaxation provides an additional source of the exchange anisotropy of approximately the same strength. The dependence of spin wave spectra on filling of Fe vacancy sites is discussed.

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