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Evidence for weak electronic correlations in Fe pnictides[1] ADAM SORINI, SLAC and Stanford, WANLI YANG, ALS, CHENG-CHIEN CHEN, BRIAN MORITZ, WEI-SHENG LEE, JIUN-HAW CHU, JIM ANALYTIS, IAN FISHER, SLAC and Stanford, B. DELLEY, FRANCOIS VERNAY, Paul Scherrer Institut, P. OLALDE-VELASCO, J. D. DENLINGER, ZAHID HUSSAIN, ALS, J. YANG, W. LU, Z. X. ZHAO, Z. A. REN, Chinese Academy of Sciences, JEROEN VAN DEN BRINK, Leiden University, Z.-X. SHEN, TOM DEVEREAUX, SLAC and Stanford — Using a combination of theoretical techniques we study the XAS and RIXS spectra of three different Fe-pnictide superconductors and parent compounds. Experimental data show that the XAS of the Fe-pnictides is similar to that of Fe metal. Motivated by this fact we analyze the size of electronic correlations, typified by Hubbard's "U" and Hund's "J", in the Fe-pnictides. Our exact diagonalization cluster calculations include explicit correlations and put an upper limit on U and J. Our relativistic Dirac atomic calculations show the relative unimportance of core-hole multiplet effects and spin-orbit coupling on the spectra. Finally, we present DFT based calculations of the XAS and XES spectra for three Fe-pnictides and Fe metal using the relativistic FEFF8 code and the WIEN2k code.

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