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X-ray spectra and electronic structure of Fe and Cu superconducting pnictides

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The results of resonant inelastic X-ray scattering (RIXS) measurements and density functional theory (DFT) calculations of Fe and Cu superconducting pnictides: $REO_{1-x}F_xFeAs$ (RE = La, Sm) [1], LiFeAs, NaFeAs [2], $CaFe_2As_2$ [3], $FeSe_x$ [4] and ACu_2B_2 (A = Ca, Sr, Ba; B = Sb, As) [5] are presented. The experimental RIXS spectra are found to be consistent with DFT calculations. Both theory and experiment show that for Fe-pnictides the Fe 3*d*-states dominate on the Fermi level and the low Hubbard *d*-band typical for correlated systems is not found. RIXS measurements at Fe $L_{2,3}$-edges show that $I(L_2)/I(L_3)$ intensity ratio is small, close to that of Fe-metal and quite different with respect to correlated FeO which is indicative of itinerant character of Fe 3*d*-electrons. The comparison of experimental RIXS spectra with LDA+DMFT (Local Density Approximation combined with Dynamical Mean-Field Theory) calculations [6] shows a good agreement between theory and experiment (with the average Coulomb repulsion $U = 3 \div 4$ eV and Hund's exchange $J = 0.8$ eV) only when Fe 3*d*-As 4*p* hybridization is taken into account. This Fe 3*d*-As 4*p* hybridization weakens electron correlations and therefore one can conclude that FeAs-based superconductors belong to weakly or moderately weakly correlated systems. It is found for Cu-pnictides that the copper 3*d* states are fully occupied and buried deep in the valence band. According to RIXS measurements at Cu $L_{2,3}$-edges, the $I(L_2)/I(L_3)$ intensity ratio in Cu-pnictides is small, comparable with that of Cu-metal and much less than in CuO and superconducting cuprates ($YBa_2Cu_3O_x$ and $YBa_2Cu_4O_8$) which indicates for weakly correlated Cu 3*d*-states.

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