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High-energy dispersion anomalies in actinide compounds T. DAS, T. DURAKIEWICZ, J.-X. ZHU, J.J. JOYCE, MATTHIAS J. GRAF, Los Alamos National Lab. — The observation of a prominent peak-dip-hump feature in the spectral weight in number of actinide compounds including Pu-115 superconductors and non-superconducting U-115 remains an unsolved problem. We have developed a first-principles intermediate coupling model to show that most aspects of these strong correlation features can be understood from the spin-fluctuation interaction.[1] The results show that a strong peak in the spin-fluctuation dressed self-energy is present around 0.5 eV in all these materials, which is mostly created by spin-orbit split 5f bands. These fluctuations couple to the single-particle spectrum and give rise to a peak-dip-hump feature, characteristic of the coexistence of itinerant and localized electronic states. Results are in quantitative agreement with photoemission spectra. Finally, we show that the studied actinides can be understood within the rigid-band filling approach, in which the spin-fluctuation coupling constant follows the same materials dependence as the superconducting transition temperature Tc. Work is supported by US DOE.

[1] T. Das. J.-X. Zhu, and M. J. Graf, arXiv:1108.0272

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