

# 5f ELECTRONS IN ACTINIDES: DUAL NATURE AND PHOTOEMISSION SPECTRA.

G. Zwicknagl

*Institut f. Mathemat. Physik, TU Braunschweig,  
Mendelssohnstr. 3, 38106 Braunschweig, Germany*

Increasing experimental evidence points towards a two-fluid model for the 5f shells in actinide-based heavy fermion compounds with some 5f electrons being localized atomic-like and others being band-like itinerant. The dual nature can explain various unusual low-energy properties of U compounds including the formation of heavy fermion and their unconventional superconductivity. The dual model, however, provides an effective Hamiltonian which is valid only for the low-energy regime. The important task is to show how this effective picture can be derived from a more microscopic description of the correlated 5f electrons. The present contribution focusses on intra-atomic correlations among the 5f electrons as a possible mechanism for orbital-selective (partial) localization. The central goal is to theoretically derive criteria and specify properties which experimentally characterize correlation-induced partial localization in actinide compounds. The ground states of extended 5f systems are analyzed treating the intra-atomic correlations within mean-field theory. The calculations confirm the qualitative results derived by exactly diagonalizing the Hamiltonians for small clusters. Correlation-induced partial localization is reflected in the 5f spectral function which can be related to photoemission data. The theoretical ansatz is based on combining ab-initio band structure calculations with typical many-body techniques like Cluster Perturbation Theory. This procedure allows for an adequate and quantitative description of the intra-atomic dynamics as reflected in the electronic properties of the 5f systems. Results for various U-based heavy fermion superconductors like UPd<sub>2</sub>Al<sub>3</sub>, its counterpart UNi<sub>2</sub>Al<sub>3</sub>, and URu<sub>2</sub>Si<sub>2</sub> will be presented emphasizing the consequences for the interpretation of experimental data. Application of the scheme to other actinides will be discussed.