

Abstract Submitted
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Quantification of U f-valence in URu₂Si₂ from 3D Bulk Fermi Surface Topology¹ JONATHAN DENLINGER, O. KRUPIN, Lawrence Berkeley Natl Lab, J.W. ALLEN, U. of Michigan, B.J. KIM, Argonne Natl Lab, K. HAULE, KYOO KIM, G. KOTLIAR, Rutgers U., J.L. SARRAO, Los Alamos Natl Lab, N.P. BUTCH, U. of Maryland, M.B. MAPLE, UC San Diego — The three-dimensional bulk Fermi surface (FS) topology of paramagnetic-phase URu₂Si₂, as measured by photon-dependent angle-resolved photoemission spectroscopy of UHV-cleaved surfaces, is presented and discussed. Complete characterization of silicon-terminated surface states using spatial dependence, surface adsorption and theoretical surface slab calculations, allows identification of the bulk electronic band structure. The bulk FS topology is shown to be distinctly different from those of both localized ThRu₂Si₂-like f-core LDA calculations (U⁴⁺) and fully itinerant LDA calculations. Key experimental FS topologies can be matched to itinerant LDA contours with suitable Fermi energy shifts that may mimic strong correlation effects not well treated in LDA. The intermediate-sized FS band topologies point to a mixed valent f-occupation between those of the two LDA calculations, $n_f \approx 2.2$ (f-core) and $n_f \approx 2.6$ (f-itinerant).

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