Electronic Structure and Compton Profiles of Tungsten

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The energy bands, density of states and Compton profiles of tungsten have been computed using band structure methods, namely the spin-polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR) approach as well as the linear combination of atomic orbitals with Hartree-Fock scheme and density functional theory. The full potential linearized augmented plane wave scheme to calculate these properties and the Fermi surface topology (except the momentum densities) have also been used to analyze the theoretical data on the electron momentum densities. The directional Compton profiles have been measured using a 100 mCi ^{241}Am Compton spectrometer. From the comparison, the measured anisotropies are found to be in good agreement with the SPR-KKR calculations. The band structure calculations are also compared with the available data.

Key words: X-Ray Scattering; Band Structure Calculations; Fermi Surface of Metals.
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