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GW **study of f-shell systems** MARK VAN SCHILFGAARDE, School of Materials, Arizona State University, ATHANASIOS N. CHANTIS, Theoretical Division, Los Alamos National Laboratory, TAKAO KOTANI, School of Materials, Arizona State University, ROBERT C. ALBERS, Theoretical Division, Los Alamos National Laboratory — We have applied the recently developed Quasiparticle Self-Consistent GW (QS*GW*) method to rare-earth metals, rare-earth compounds, and actinide metals. Comparison with the available experimental data shows that this method can successfully describe the electronic structure of these materials within a unified ab-initio theoretical framework. Through this approach we can examine the approximations that enter into the LDA+U method and show ways of improving its implementation. Based on the QS*GW* bands, a discussion of the role of electronic correlations on the band structure of uranium and plutonium will be presented. Finally, we uncover a completely new effect: a first-order metal-insulator transition in GdN, which is driven by dielectric function changes. This result may explain the ambiguities in the experimental data obtained for this material.

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