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LDA+Gutzwiller and Topological Maters in Rare-Earth and Actinide Compounds: Competition and Cooperation between localised and Itinerant Natures of the Electrons in Solids

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This presentation explores the complex interplay between localized and itinerant electronic behaviors in rare-earth and actinide compounds, focusing on the role of strongly correlated $4f$ and $5f$ electrons in stabilizing topological quantum states. The dual nature of f-electrons—simultaneously atomic-like and band-like—poses significant challenges for conventional electronic structure methods. The talk highlights the **LDA+Gutzwiller** approach as an effective framework for capturing both the localized multiplet physics and the renormalized quasiparticle bands. Using this method, several key material systems are examined, including **mixed-valent topological insulators** (e.g., SmB_6, YbB_6, YbB_{12}), **non-centrosymmetric heavy-fermion Weyl semimetals** (e.g., $CeRu_4Sn_6$), and **rare-earth magnetic topological materials** (e.g., EuB_6, $EuIn_2As_2$, U_3As_4). The discussion demonstrates how strong correlations, magnetic order, and band topology cooperate to produce exotic phenomena such as topological surface states, Fermi arcs, and higher-order topological insulating phases, offering new pathways for engineering correlated topological matter.