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The f-electron challenge: localized and itinerant states in lanthanide oxides united by GW@LDA+U MATTHIAS SCHEFFLER, HONG JIANG, RICARDO I. GOMEZ-ABAL, FHI, Berlin, Germany, PATRICK RINKE, UC Sant Barbara, CA 93106 — Understanding the physics of f-electron systems, characterized by the competition between itinerant (delocalized) and highly localized f-states, is regarded as a great challenge in condensed-matter physics today. As a first step towards a systematic *ab initio* understanding of f-electron systems, we apply many-body perturbation theory in the G_0W_0 approach based on LDA+U ground state calculations (G_0W_0@LDA+U) to a selected set of lanthanide oxides (CeO_2 and Ln_2O_3 (Ln=lanthanide series)). These compounds have important technological applications, in particular in catalysis and microelectronics. We demonstrate good agreement between the G_0W_0 density of states (DOS) and experimental spectra for CeO_2 and Ce_2O_3. For the whole Ln_2O_3 series G_0W_0@LDA+U reproduces all main features found for the optical experimental band gaps. Inspection of the DOS reveals that the relative positions of the occupied and unoccupied f-states predicted by G_0W_0 confirm the experimental conjecture derived from phenomenological arguments.

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