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$_2$O$_3$ (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$_2$O$_3$. For the whole Ln$_2$O$_3$ 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.