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Dielectric properties of high-k oxides: Theory and experiment for Lu2O3 EMILIANO BONERA, Laboratorio Nazionale MDM-INFM, GIOVANNA SCAREL, Laboratorio Nazionale MDM-INFM, MARCO FANCIULLI, Laboratorio Nazionale MDM-INFM, PIETRO DELUGAS, INFM-SLACS Universit di Cagliari, VINCENZO FIORENTINI, INFM-SLACS Universit di Cagliari — The quest for a dielectric for the replacement of silica in Si-based devices has focused the attention of the scientific community on the class of high dielectric constant (κ) insulators. In this work we unfold the physical origin of κ and its direct connection with lattice dynamics and polarizability in these materials, analyzing the specific case of Lu_2O_3 in its ground-state bixbyite structure with a combined experimental and theoretical analysis. The vibrational dielectric function of Lu_2O_3 thin films grown by atomic-layer deposition was studied by infrared transmission and reflection-absorption spectroscopies, selectively accessing transverse and longitudinal optical frequencies. The static dielectric constant was extracted analyzing the infrared response. We also present first-principles density-functional linear-response calculations, which are in close agreement with experiment, and provide insight into the microscopic nature of vibrational spectra and dielectric properties.

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