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Dielectric and vibrational properties of crystalline and amorphous high-k lanthanum aluminate PIETRO DELUGAS, VINCENZO FIORENTINI, ALESSIO FILIPPETTI, INFM-SLACS and University of Cagliari, Italy — We present ab-initio density-functional and self-interaction-corrected calculations on the structure, long-wavelength IR and Raman vibrational modes, and static dielectric properties of the high-k oxide $LaAlO_3$, including the recently-observed dielectric anisotropy. The orientation-averaged dielectric constant k=23.3 in the crystal is in good agreement with experiment, and it is dominated by lattice response. We then evaluate by finite-field linear-response calculations the dielectric and polarization properties of an amorphous sample generated by ab initio molecular dynamics. The dielectric response is largely analogous to that of the crystal, due to the conservation of the main IR active modes and La anomalous charges due to a quite sharp Al-O and La-O short-range order. We find it important to calculate the dynamical charges by a self-interaction-corrected scheme, bringing about a $\sim$15% improvement over DFT.

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