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**Dielectric and vibrational properties of crystalline and amorphous high-k lanthanum aluminate** PIETRO DELUGAS, VINCENZO FIORENTINI, ALESSIO FILIPPETTI, SLACS-CNR and University of Cagliari, Italy — High-k oxides are the focus of intense research for their applications in MOS and FLASH devices. A material currently in focus is $LaAlO_3$, with a dielectric constant of 23-24 in the crystal phase, and similar values of around 20-22 in the amorphous phase (although values as low as 15 have also been reported). We have studied $LaAlO_3$ in both phases [1] to identify possible reasons for this apparent conservation of the dielectric properties upon amorphization. Amorphous samples were generated by melt-and-quench using a combination of pair potentials and ab initio dynamics. The linear response density-functional perturbation-theory approach was used to study dynamical response and phonons. We indeed find a large dielectric constant ( 24) in the amorphous: the rationale is that the expected reduction of the anomalous effective charges is compensated by the appearance of new low-frequency (weakly) IR-active modes, whose character is a mixture of La translations (IR in the crystal) and Al-O octahedra rotations (Raman in the crystal). A similar behavior is expected in any rare earth aluminate exhibiting a similar perovskite-related structure (e.g. scandates).
1) P. Delugas, V. Fiorentini, and A. Filippetti, Phys. Rev. B 71, 134302 (2005), and to be published.

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