Abstract Submitted
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Hybrid functional calculations for the electronic properties of $LaAlO_3$[1] JIMMY-XUAN SHEN, Department of Physics, UCSB, California 93106-9530, USA, ANDRÈ SCHLEIFE, Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, Livermore, California 94550, USA , ANDERSON JANOTTI, Materials Department, UCSB, Santa Barbara, California 93106-5050, USA , CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, California 93106-5050, USA — The perovskite $LaAlO_3$ is a wide-band-gap (5.5–6.5 eV) insulator of high interest in both applied and fundamental research. On the applied side, $LaAlO_3$ has been considered a candidate to replace SiO_2 as a gate dielectric in field-effect transistors due to its high dielectric constant (23–25) and near-perfect lattice matching with Si ($< 1\%$). On the fundamental science side, two-dimensional electron gases (2DEGs) with high carrier density have been observed at the interface of $LaAlO_3$ and $SrTiO_3$. The origin of the 2DEG and the dependency of its density on the thickness of the $LaAlO_3$ top layer have been highly debated. Interestingly, many of the basic electronic properties of $LaAlO_3$ are still poorly understood. For example, measurements of the band gap vary by as much as 1 eV. Here, we report the electronic structure of $LaAlO_3$ using density functional calculations with a hybrid functional. We compute the electronic structure and the dielectric function of bulk $LaAlO_3$ in the rhombohedral and cubic phases, and compare the optical properties with experiments.

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