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Dielectric tensors of high-k *Pbnm* perovskites from first principles
SINISA COH, DAVID VANDERBILT, Rutgers University — Among the materials under consideration for future high-k dielectrics in MOSFET and other microelectronic devices are several perovskites having space group *Pbnm*. Among these are $LaLuO_3$, $SrBO_3$ (B = Zr, Hf), $AScO_3$ (A = La, Pr, Nd, Sm, Gd, Tb, Dy), and $LaB_{1/2}Zr_{1/2}O_3$ (B = Ca, Mg) (with lower symmetry), which are all compatible with growth on silicon and can have higher dielectric constants than HfO_2.[1,2] Using first-principles DFT methods with ultrasoft pseudopotentials and GGA energy functionals, we compute the dielectric tensors, structural properties, and phonon spectra of these materials. We analyze the dependence of these properties on chemical composition, and compare with experiments where possible. We also focus on correlation between dielectric tensor anisotropy and octahedra rotation angles.

[1]D. G. Schlom, S. Guha, S. Datta, MRS Bull. **33**, 1017 (2008).
[2]Thin Films and Heterostructures for Oxide Electronics, S. B. Ogale, Ed. (Springer, New York 2005), pp. 31-78.

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