

# Si-compatible candidates for high- $\kappa$ dielectrics with the *Pbnm* perovskite structure

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Received 26 April 2010; published 3 August 2010

We analyze both experimentally (where possible) and theoretically from first principles the dielectric tensor components and crystal structure of five classes of *Pbnm* perovskites. All of these materials are believed to be stable on silicon and are therefore promising candidates for high- $\kappa$  dielectrics. We also analyze the structure of these materials with various simple models, decompose the lattice contribution to the dielectric tensor into force constant matrix eigenmode contributions, explore a peculiar correlation between structural and dielectric anisotropies in these compounds and give phonon frequencies and infrared activities of those modes that are infrared active. We find that CaZrO<sub>3</sub>, SrZrO<sub>3</sub>, LaHoO<sub>3</sub>, and LaYO<sub>3</sub> are among the most promising candidates for high- $\kappa$  dielectrics among the compounds we considered.

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URL:

<http://link.aps.org/doi/10.1103/PhysRevB.82.064101>

DOI:

10.1103/PhysRevB.82.064101

PACS:

77.22.-d, 77.55.df, 85.50.-n

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