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First Principle Based Computation of Pyroelectricity in LiNbO3

Q. PENG[1], Center for Statistical and Theoretical Condensed Matter Physics, Zhejiang Normal University, Jinhua 321004, China, R.E. COHEN, Carnegie Institution, 5251 Broad Branch Road NW, Washington, D.C., 20015,USA — Pyroelectricity is of current interest since the discovery of particle acceleration of aqueous ions from changes in temperature at pyroelectric surfaces sufficient to generate hard X-rays[1] as well as neutrons via fusion[2]. We computed the pyroelectric coefficients in LiNbO3 from molecular dynamic simulation with DLPOLY using a shell model potential fitted to Density Functional Theory computations results. The potential was constructed by fitting energies and forces, as well as phonon frequencies and eigenvectors, Born effective charges, and dielectric constants computed from density functional perturbation theory using ABINT. The secondary pyroelectric effect is computed from density functional theory. The spontaneous polarizations were calculated using the Berry phase method. The coefficient of thermal expansivity, elastic moduli, elastic compliances, piezoelectric stress constants and piezoelectric strain constants are computed by linear response and lattice dynamics computations. [1] J. D. Brownridge and S. Raboy, Journal of Applied Physics 86, 640 (1999). [2] B. Naranjo, J. Gimzewski, and S. Putterman, Nature 434, 1115 (2005).

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