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First-principle calculation of elastic and piezoelectric tensors and zone center phonons in $LiGaO_2$ ADISAK BOONCHUN, WALTER LAMBRECHT, Case Western Reserve University — The elastic, piezoelectric tensor and vibrational modes of $LiGaO_2$ have been studied by means of first-principles density functional calculations using the pseudopotential linear-response approach in the local density approximation. The lattice constants of the orthorhombic structure are obtained in agreement with experiment to better than 2%. The calculated dielectric constants in the a, b, and c directions are obtained to be about 6.37, 6.98, and 7.44, comparing to 6.5, 7.0 and 8.3 from experimental data. Elastic constant were calculated from the second derivatives of total energy versus strain while piezoelectric constants were calculated from the second mixed derivatives of total energy versus electric field and strain. Our results for both elastic constants and piezoelectric constants agree well with experimental results. Using the calculated oscillator strengths and high-frequency dielectric tensor, the infrared reflectivity for the a_1,b_1 and b_2 modes are obtained in excellent agreement withexperimental data both in terms of peak positions and relative peak heights.

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