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First-principles study of $LiAlO_2$ in tetrahedrally and octahedrally coordinated structures PHILLIP POPP, WALTER LAMBRECHT, Case Western Reserve University — Ultrawide-band gap (UWBG) semiconductors (band gap >4 eV) have many potential interesting applications, such as in high-power electronics and deep-UV optoelectronic devices. $LiAlO_2$ is a candidate material for UWBG semiconductors. This project is a first-principles electronic structure study of $LiAlO_2$, focusing on band gap/band structure, bulk moduli of common crystal structures, and transition pressures between different structures. Specifically, we compare the tetragonal γ and orthorhombic β structures (both tetrahedrally coordinated) with the octahedrally coordinated R-3m α structure. We calculate these properties using the density functional theory (DFT)-based linearized muffin tin orbital (LMTO) and pseudopotential plane wave methods. We find that the tetrahedrally bonded structures have slightly lower energy than the octahedral one and a transition to the octahedral phase occurs near 1.5 GPa.

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