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DFT Predictions of Electronic, Transport, and Bulk Properties of Cubic Antifluorite A_2B Compounds (A= Li, Na, B= O,S,Se) [1] YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, DIOLA BAGAYOKO, Department of Physics Southern University and AM College, Baton Rouge, LA 70813 — We present results from *ab-initio,* self-consistent calculations of electronic, transport, and bulk properties of cubic antifluorite (anti-CaF_2) compounds A_2B (A = Li, Na, B = O, S, Se). Our computations employed the local density approximation (LDA) potential of Ceperley and Alder and the linear combination of atomic orbital (LCAO) formalism. The implementation of the LCAO formalism followed the Bagayoko, Zhao, and Williams method, as enhanced by Ekuma and Franklin (BZW-EF). Consequently, our calculations search for and attained the ground states of the systems under study, as required by DFT; our results therefore possess the full, physical content of DFT. We discuss band structures, band gaps, and related properties of these materials, including calculated, total and partial densities of states (DOS and PDOS), effective masses of charge carriers, equilibrium lattice constants, and the bulk moduli of cubic antifluorite compounds A_2B (A = Li, Na, B = O, S, Se). Our results are predictions in some cases, due to the lack of experimental data.

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