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First principles investigation of structural, dynamic, electronic and optical properties of Barium seleno-germanate Ba₂GeSe₄

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Ternary and quaternary chalco-germanates and stannates have a rich structural chemistry. Experimental studies of their nonlinear optical properties have been reported, but there are few published computational studies on their structural, dynamic, electronic and optical properties. In this work, we investigate the structural, dynamic, electronic and optical
properties of Ba₂GeSe₄ using Density Functional Theory (DFT) and post-DFT many body perturbation theory. The ground state energy and properties, including equilibrium lattice parameters, bulk modulus, band gap and phonon dispersion were calculated at the DFT level of approximation. The fundamental gap was determined at the post DFT G₀W₀ level of approximation while optical absorption was determined within the Bether-Salpeter Equation approximation. The ground state energy, mechanical and phonon dispersion results show that Ba₂GeSe₄ is a stable compound while the calculated optical absorption results show that it is a wide band gap material that is well-situated for photon absorption in visible range.

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