# The electronic structure and optical properties of $YGa_2$ superconductor

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The electronic structure and optical properties of the intermetallic compound $YGa_2$ have been investigated using first-principles calculations. The calculations were performed within the framework of density functional theory (DFT) employing the projector augmented-wave (PAW) method [1], as implemented in the Vienna Ab-initio Simulation Package (VASP) [2]. The exchange-correlation effects were described using the generalized gradient approximation (GGA) in the Perdew–Burke–Ernzerhof (PBE) parametrization [3]. The electronic self-consistent calculations were converged to an energy accuracy of $10^{-8}$ eV. Brillouin-zone integrations were carried out using the tetrahedron method with an $8 \times 8 \times 12$ Monkhorst–Pack k-point mesh [4]. The optical anisotropy of $YGa_2$ was analyzed by calculating the frequency-dependent optical functions, including the refractive index and dielectric function along the principal crystallographic directions. The calculated electronic band structure and optical spectra are presented and discussed. Furthermore, the obtained results are compared with the reported theoretical data for $MgB_2$ and $AlB_2$ [5], which crystallize in the same $AlB_2$-type hexagonal structure (space group $P6/mmm$).

**References**

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