Abstract Submitted
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Dielectric, magnetic, magneto-optical and nonlinear optical properties of ferroelectric ferromagnetic semiconductor $BiMnO_3$ from first-principles calculations GUANG-YU GUO[1], HAI-QING LIN, Department of Physics, Chinese University of Hong Kong, Shatin, Hong Kong — $BiMnO_3$ is a biferroic (ferroelectric and ferromagnetic) semiconductor, and hence a member of the family of multiferroic materials. In order to gain a full understanding of its interesting properties such as biferroic behavior, we have calculated from first-principles the electronic structure, exchange coupling, linear and non-linear optical susceptibilities as well as magneto-optical Kerr rotation of $BiMnO_3$. The calculations are based on density functional theory with generalized gradient approximation plus on-site Coulomb correlation (GGA+U). The all-electron full potential linearized augmented plane wave (FLAPW), frozen core full potential projector augmented wave (PAW), and also all-electron tight-binding linear muffin-tin orbital methods (TB-LMTO) are used. In this contribution, we will present and analyze the obtained exchange coupling parameters, magneto-optical Kerr rotation spectra, dielectric constants and second-harmonic generation coefficients.

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