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Role of Nd and Gd Dopants on Multiferroic Behavior of $BiFeO_3$ — A First-Principle Study

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Electronic band structure, ferroelectric, and magnetic properties of multiferroic Bi1.xRExFeO$_3$ ($x = 0$, 0.16, 0.32, 0.5; $RE =$ Nd and Gd) doped compounds have been investigated using TB-mBJ semi-local (Tran–Blaha modified Becke–Johnson) potential approximation method and WIEN2k code. As spin.orbit coupling (SOC) influences several properties of these materials, SOC corrections were also included in the present study. On the basis of varying band gap values, it has been concluded that the leakage current might have decreased with increasing dopant concentration. It has been concluded from the charge density studies that stereo chemically active $6S^2$ lone-pair electrons are present at Bi sites and they might be responsible for the displacements of Bi atoms from the centrosymmetric to the non-centrosymmetric structure position leading to the exhibition of ferroelectricity. It was also observed that magnetic moments of iron ions are not integral values probably due to hybridization of Fe electrons with neighboring O ions. To understand ferroelctric properties of these compounds, the real and imaginary parts of the dielectric functions were obtained at ambient conditions and were analyzed using TB-mBJ + SOCpotentials. Finally, it has been concluded that the results obtained in the present investigations may be useful in predicting the properties of bismuth ferrite for possible applications in industry.

Keywords: multiferroics, TB-mBJ exchange potential, charge density, spin–orbit coupling (SOC),