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First-principle calculations of electronic structure of bismuth ferrate and manganate with the mullite structure JEN-CHANG CHEN, CHING-MING WEI, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, 10617, Taiwan — We applied ab initio total-energy calculation to study the electronic structure of $Bi_2Fe_4O_9$ and $Bi_2Mn_4O_{10}$ single crystals. Both crystals are orthorhombic with the centro-symmetric structure and belong to the mullite-type material. Most of bismuth-based oxides exhibit good ferroelectricity, pyroelectricity and piezoelectricity. However, little researches of electronic structure and properties have been done on the bismuth ferrate and bismuth manganate. In this study, the band structure, density of state, partial density of state and magnetic moment of both bismuth ferrate and bismuth manganate at zero Kevin were calculated. The effect of Fe and Mn atom within the structure were discussed. The phase stability of these two crystals was also examined.

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