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**Computational study of the ferromagnetic and ferroelectric properties of ($Bi_2Mn\ NiO_6)_4$.** LEONARD KLEINMAN, B.R. SAHU, ADRIAN CIUCIVARA, University of Texas at Austin — Using the VASP PAW code with the GGA and including spin-orbit coupling and allowing for non collinear magnetization, we performed electronic structure calculations for the multiferroic crystal, ($Bi_2Mn\ NiO_6)_4$. The lattice angle and lattice constants are in excellent agreement with experiment. The magnetization is 4.94 $\mu_B$. The polarization, for which there is no experimental value, is 16.84 $\mu Ccm^{-2}$. Inverting the positions of all the atoms we iterated to convergence. The magnetization did not change and the total energy was also unchanged. Thus we conclude that the polarization and magnetization are uncoupled and ($Bi_2Mn\ NiO_6)_4$ is unlikely to have any device applications.

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