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Huge spin-driven polarizations at room temperature in bulk $BiFeO_3$[1] JUN HEE LEE, RANDY FISHMAN, Oak Ridge National Laboratory — Although $BiFeO_3$ is one of the most investigated multiferroics, its magnetoelectricity and spin-driven polarizations are barely understood on an atomistic level. By combining a first-principles approach with a spin-cycloid model, we report hidden but huge spin-driven polarizations at room temperature in bulk $BiFeO_3$. One of the polarizations reaches ~ 0.03 C/m^2, which is larger than any other spin-driven polarization in a bulk material by one order of magnitude. By comparing our results with intrinsic measurements such as neutron scattering, Raman spectroscopy, IR directional dichroism, and high magnetic-field measurements, we disentangle all the hidden spin-driven polarizations due to exchange-striction, spin-current, and single-ion-anisotropy. We find that the broken inversion symmetries of the $R3c$ structure of $BiFeO_3$ induce the strong response of the magnetic couplings to an electric field and are responsible for the associated huge spin-driven polarizations.

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