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Quantum Monte Carlo calculations of BiFeO3[1] LUCAS K. WAGNER, DAVID SULOCK, LUBOS MITAS, North Carolina State University — Multiferroic Bismuth Ferrite (BiFeO3) exhibits both ferroelectricity and antiferromagnetism, possibly enabling a connection between the two effects in the same material. While its antiferromagnetic character is relatively well-understood, experimental measurements of the spontaneous polarization vary significantly over two orders of magnitude, from 0.06 C/m^2 to 1.50 C/m^2. We cary out accurate quantum Monte Carlo calculations to estimate the cohesion energy and the ferroelectric distortion well depth. We discuss the mechanisms proposed to understand the variations of polarization experimental data in the light of our quantum Monte Carlo results.

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