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Frustrated Antiferroelectricity in a Room-Temperature Ferrimagnet: Promising Candidate Toward Multiple State Memory PANSHUO WANG, HONGJUN XIANG, Department of Physics, Fudan University, Shanghai 200433, P. R. China — Frustration refers to the presence of competing forces that cannot be simultaneously satisfied. However, geometrical frustration in ferroelectrics is highly unusual. Here we show from first-principles calculations that the M-type hexaferrite $BaFe_{12}O_{19}$ exhibits frustrated antiferroelectricity, and hence resolve the experimental controversy on the local structure of the trigonal bipyramidal (TBP) site. Due to the electrostatic interaction, the high-spin Fe^{3+} ions at the TBP sites are displaced from the mirror-plane sites to generate local dipole moments along the c axis. Because of the dipole-dipole interactions, the ground state of $BaFe_{12}O_{19}$ is a(2×1) chain-like antiferroelectric (AFE) phase. Our work indicates that the ferroelectric state is metastable and can be reached by applying an external electric field to the AFE state, and that the FE state can be made stable at room temperature by element substitution or strain engineering. Thus M-type hexaferrites not only provide platform for studying the new physics of the frustrated antiferroelectricity, but also are promising candidates for realizing multiple state memory devices based on the coexistence of the room temperature polar order and strong ferrimagnetic order.

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