Highlights

RESEARCH AREA 2 - **Functional and Complex Materials for Innovative Electronics and Sensing** - 2022

"γ-BaFe2O4: a fresh playground for room temperature multiferroicity"

Fabio Orlandi 1 , Davide Delmonte 2 , Gianluca Calestani3 , Enrico Cavalli3 , Edmondo Gilioli2 , Vladimir V. Shvartsman 4 , Patrizio Graziosi5 , Stefano Rampino2 , Giulia Spaggiari2,6, Chao Liu7,8, Wei Ren 7 , Silvia Picozzi8 , Massimo Solzi 6 , Michele Casappa 2,3 & Francesco Mezzadri 2,3

1 ISIS Facility, Rutherford Appleton Laboratory, Harwell Campus, Didcot OX11 0QX, UK.
2 IMEM-CNR, Parco Area delle Scienze 37/A, 43124 Parma, Italy.
3 Department of Chemistry, Life Sciences and Environmental Sustainability, University Parma, Parco Area delle Scienze 17/A, 43124 Parma, Italy.
4 Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), Univ. Duisburg-Essen, 45141 Essen, Germany.
5 CNR-ISMN, Via P. Gobetti 101, 40129 Bologna, Italy.
6 Department of Mathematical, Physical and Computer Sciences, University of Parma, Parco Area delle Scienze 7/A, Parma, Italy.
7 Physics Department, International Center of Quantum and Molecular Structures, Materials Genome Institute, State Key Laboratory of Advanced Special Steel, Shanghai Key Laboratory of High Temperature Superconductors, Shanghai University, Shanghai 200444, China.
8 Consiglio Nazionale delle Ricerche (CNR-SPIN), Unità di Ricerca presso Terzi c/o Università "G. D'Annunzio", 66100 Chieti, Italy

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Multiferroics, showing the coexistence of two or more ferroic orderings at room temperature, could harness a revolution in multifunctional devices. However, most of the multiferroic compounds known to date are not magnetically and electrically ordered at ambient conditions, so the discovery of new materials is pivotal to allow the development of the field. In this work, we show that BaFe2O4 is a previously unrecognized room temperature multiferroic. X-ray and neutron diffraction allowed to reveal the polar crystal structure of the compound as well as its antiferromagnetic behavior, confirmed by bulk magnetometry characterizations. Piezo force microscopy and electrical measurements show the polarization to be switchable by the application of an external field, while symmetry analysis and calculations based on density functional theory reveal the improper nature of the ferroelectric component. Considering the present findings, we propose BaFe2O4 as a Bi- and Pb-free model for the search of new advanced multiferroic materials.

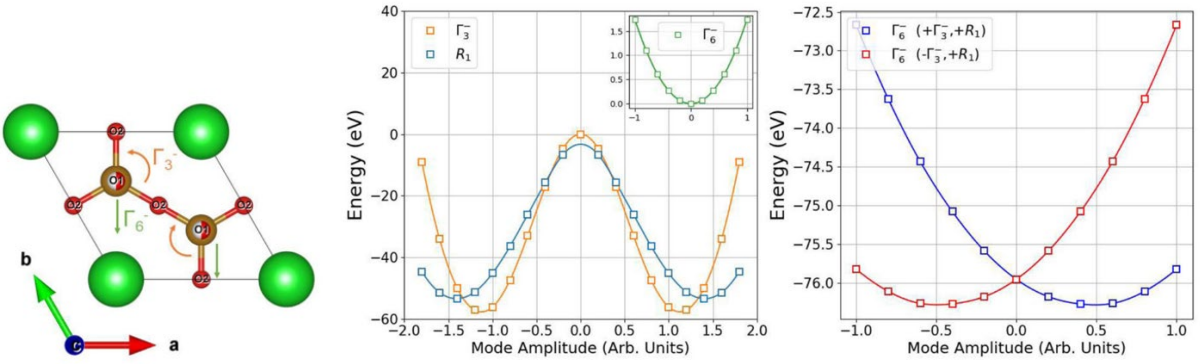

Fig.1 - Left panel: The orange and green arrows denote the displacements due to the Γ3- and Γ6- modes. Central panel: DFT total energies as a function of mode amplitudes, considering only the Γ3− (orange line) and R1 (blue line) modes. The inset shows the total energy behavior, when activating only the Γ6− mode. Right panel: DFT total energies obtained by changing the Γ6− amplitude, in the presence of the R1 mode amplitude frozen to its positive minimum and the Γ6- mode frozen to the positive minimum (blue points) and to the negative minimum (red points).