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Green synthesis of BiFeO3 using natural fuels: optical and structural characterization and magnetoelectric response measurement

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Introduction

$BiFeO_3$ (BFO) is a type-I multiferroic material exhibiting ferroelectric and G-type antiferromagnetic ordering above room temperature. It presents a ferroelectric T_Curie≈1103 K and an antiferromagnetic T_Néel ≈ 643 K.
Its ferroelectricity originates mainly from the stereochemically active Bi^{3+} $6s^2$ lone pair, while magnetism arises from Fe^{3+} spin ordering. The coexistence of these ferroic orders enables magnetoelectric coupling, making BFO a promising material for multifunctional devices, magnetic sensors, and spintronic applications.

BFO samples were synthesized via microwave-assisted combustion using glycine, citric acid, green coffee, and unroasted cocoa extracts. The resulting powders exhibited a rhombohedral perovskite structure (R3c), with crystallite sizes of 23–43 nm, and band gaps of 2.17–2.21 eV. After sintering at 700 °C, ceramic pellets prepared with citric acid showed the highest $BiFeO_3$ phase fraction (80.5%) and magnetoelectric voltage coefficient (0.2067 mV cm^{-1} Oe^{-1}), highlighting the influence of phase composition and particle size on magnetoelectric performance.

Objective

To explore the use of bio-derived and alternative combustion agents as a strategy to reduce reliance on conventional synthetic fuels in $BiFeO_3$ synthesis, while evaluating their influence on material properties among these their magnetoelectric performance.

Results and discussion

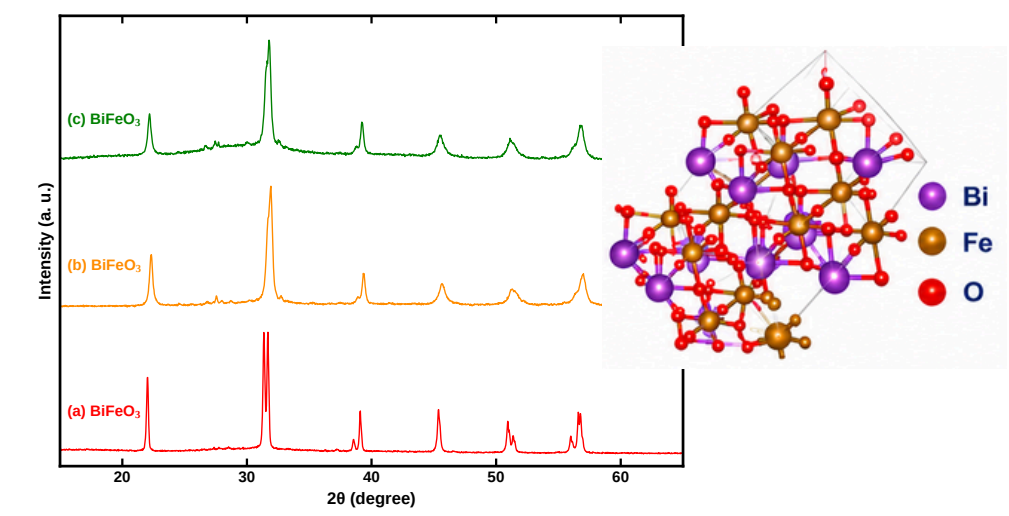
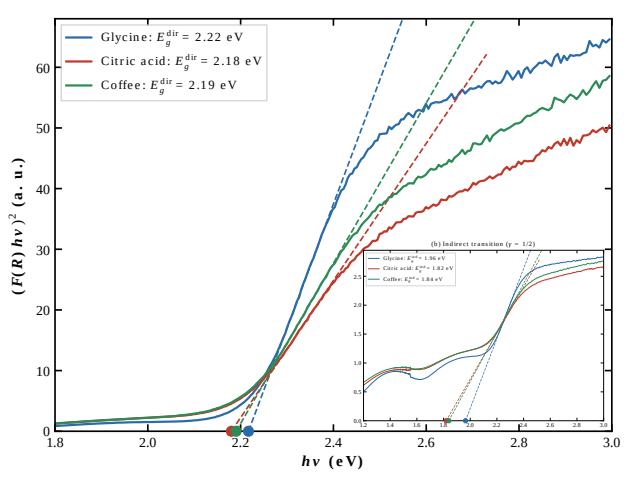
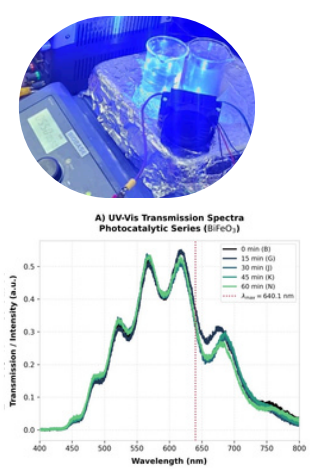


Figure 1. XRD patterns of combustion-synthesized $BiFeO_3$ using (a) glycine, (b) coffee, and (c) citric acid as fuels.

Sample	Glycine	Citric acid	Coffee extract
D_{avg} (nm)	**43.2 ± 2.1**	23.2 ± 1.5	24.3 ± 1.7

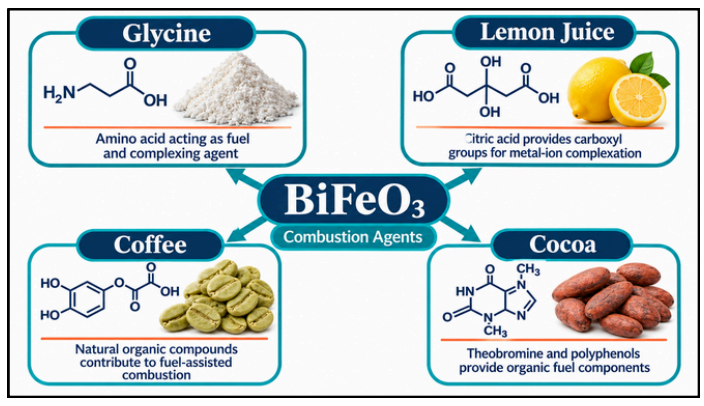
Diffractograms confirm the formation of the rhombohedral perovskite phase $BiFeO_3$ (space group R3c), with no significant peak shifts or appreciable changes in lattice parameters. The glycine-synthesized sample exhibits narrower and better-defined reflections, whereas those obtained using citric acid and coffee extract show greater peak broadening, suggesting differences in crystallite size and lattice microstrain associated with the fuel agent.





The samples exhibit a direct band gap of 2.18–2.22 ± 0.01 eV (λ≈ 440 a 590 nm), indicating optical absorption within the visible region of the electromagnetic spectrum. These results suggest that the synthesis agent preserves the material's electronic structure while promoting efficient solar radiation harvesting.

Methodology





The materials were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), EDX spectroscopy, and UV-Vis-NIR diffuse reflectance spectroscopy. Subsequently, the powders were uniaxially pressed and sintered at 700 °C for 2 hours to measure the magnetoelectric voltage coefficient (αE) using equipment developed by our research group.

SEM micrographs reveal a strong dependence of the microstructure on the chelating agent. Glycine produces rounded, porous agglomerates (≈1–2 μm) composed of quasi-spherical particles (0.2–0.5 μm). In contrast, citric acid and coffee extract yield irregular, angular fragments (0.15–0.5 μm) grouped into compact clusters.

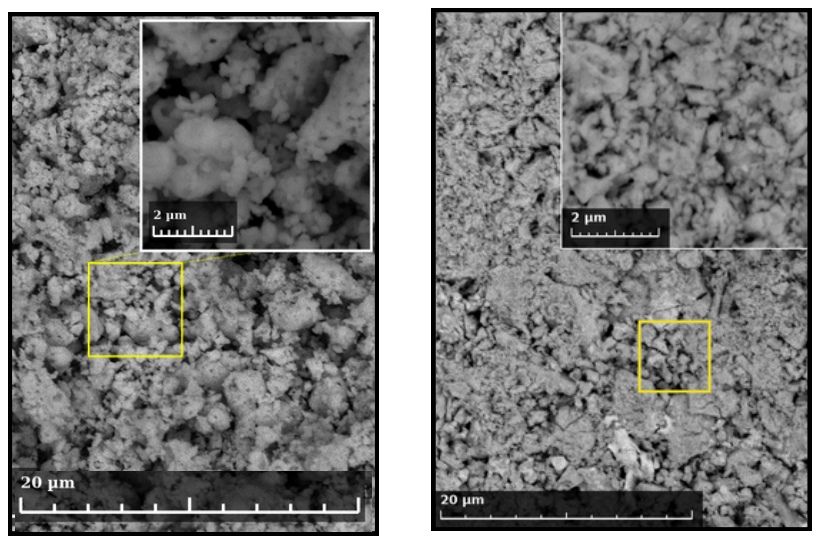
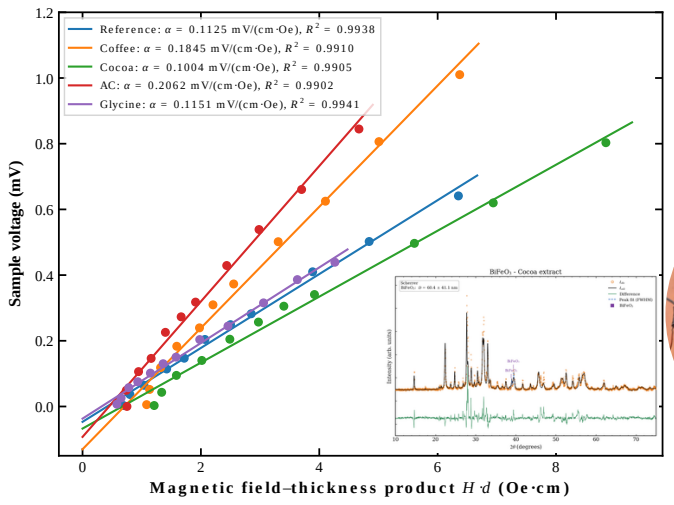
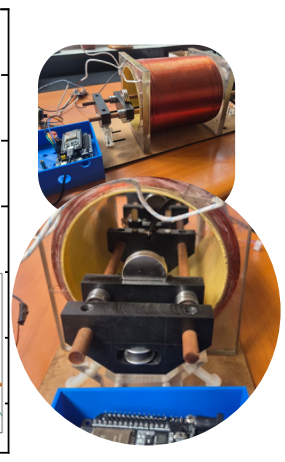


Figure 2. SEM micrographs of $BiFeO_3$ synthesized using glycine (left panel) and citric acid (right panel) .

Particle size analysis yielded average diameters of 148.55 ± 29.11 nm (glycine), 123.38 ± 26.46 nm (coffee), and 102.41 ± 22.06 nm (citric acid). the particle sizes are approximately 3.4–4.4 times larger than the crystallite sizes estimated by XRD, suggesting that the particles consist of multiple crystallites, forming a polycrystalline structure and a higher grain-boundary density in the samples synthesized using alternative fuels.

Magnetoelectric coupling coefficient ➡ $\alpha_E = \frac{\Delta E}{\Delta H} = \frac{\Delta V}{t \cdot \Delta H}$





Measured magnetoelectric coupling coefficient (αE) ranged from 0.10 to 0.21 mV/(cm·Oe), exhibiting high linearity (R^2 ≈ 0.99). The response may be influenced by crystallite size, grain boundaries, and secondary phases, which can affect the magnetoelectric coupling. The obtained values are of the same order of magnitude as those reported in the literature (0.3–0.6 mV/(cm·Oe)).

Conclusions

Rhombohedral perovskite BFO (R3c) was successfully synthesized via microwave-assisted combustion using different fuels (glycine, citric acid, and green coffee extract), establishing a sustainable fabrication route. The samples exhibit structural, morphological, and optical properties in strong agreement with literature, notably polycrystalline nanoparticles (102–149 nm), crystallite sizes ranging from 23.2 to 43.2 nm, high grain-boundary density, and direct band-gap transitions (2.18–2.22 eV) suitable for visible-light photoactive applications. Furthermore, an open-source instrumental system was developed and validated, yielding initial experimental measurements of the Magnetoelectric coupling coefficient (αE) within the expected order of magnitude for polycrystalline BFO

References and Acknowledgments

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