**Structure-based magneto-dielectric response in Zn and V Co-doped NiFe2O4 for magnetic and spintronic applications**

Md. Sarowar Hossaina,\*, Sagar Duttab, Md. Rabiul Hassanc,d, Ejaj Tarife , M.D.I. Bhuyanf , Angkita Mistry Tamaa, M.D. Hossaind,g, Gourab Kumar Royb

aDepartment of Physics, American International University-Bangladesh, Dhaka 1229, Bangladesh

bInstitute of Natural Sciences, United International University, United City, Madani Ave, Dhaka 1212, Bangladesh

cRooppur Nuclear Power Plant, Pabna 6620, Bangladesh

dDepartment of Physics, Khulna University of Engineering & Technology, Khulna 9203, Bangladesh

eDepartment of Chemistry, GLA University, Mathura, 17 km Stone, NH-19, Mathura-Delhi Road, Mathura, UP, PO Chaumuhan 281406, India

fDepartment of Physics, Mawlana Bhashani Science and Technology University, Santosh, Tangail 1902, Bangladesh

gDepartment of Computer Science and Engineering, Northern University of Business & Technology Khulna, Khulna 9100, Bangladesh

\*Corresponding author. E-mail addresses: sakil\_phy@aiub.edu, sakil\_phy@yahoo.com

**Abstract**

This study implemented the sol-gel method to synthesize NiFe2O4 (NFO) and Ni0.6Zn0.4Fe1.94V0.06O4 (NZFVO) nanoparticles. X-ray diffraction (XRD) with Rietveld refinement confirmed cubic spinel structures, while FESEM and TEM showed that dopants caused lattice distortion, leading to larger grains and crystallites in NZFVO. First- principles calculations show a reduced direct bandgap and conduction band splitting in NZFVO, attributed to strong d–p orbital hybridization. Mulliken population analysis indicates off-center cationic displacements and increased covalency, further supporting the observed dielectric and magnetic behavior. Dielectric measurements confirmed lower permittivity and loss in NZFVO, indicating its suitability for low-loss spintronic devices. Magnetic characterization shows enhanced saturation magnetization, lower coercivity, and reduced Curie temperature (Tc) in NZFVO, resulting from optimized cation distribution and weakened anisotropy. Therefore, NZFVO, with high saturation magnetization (~72.4 emu/g) and low coercivity (~6.6 Oe), is well-suited for low-field detection, magnetic biosensing, and room-temperature sensing. Its reduced bandgap and strong d-p hybridization enable spin-dependent conduction, while moderate conductivity and low resistivity make it a promising channel material for spin-based transistors and logic devices.

**Keywords:** Spinel ferrite Mulliken population analysis Density of states Dielectric relaxation Magnetic anisotropy