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Anomalous enhancement of Neel temperature and magnetic coupling for $\mathbf{Bi}_{0.9}\mathbf{Ca}_{0.1}\mathbf{FeO}_{3-\delta}$ and $\mathbf{Bi}_{0.9}\mathbf{Pb}_{0.1}\mathbf{FeO}_{3-\delta}$ GOPESHMWAR-DHAR DWIVEDI, KUNG-SHANG YANG, BO-YU CHEN, HSIUNG CHOU¹, Dept. of Physics ,NSYSU, Kaohsiung 804, Taiwan — Temperature dependent neutron diffraction patterns of the Ca-doped BiFeO₃ and Pb-doped BiFeO₃ show that their Neel temperatures (T_N) increase to 710 K and 680 K, while pure BiFeO₃ has a T_N ~643 K. X-ray absorption spectra clearly shows that there is no evidence of mixed valence states despite divalent cation doping in trivalent Bi-sites. X-ray photoemission spectroscopy study revealed that divalent doping has introduced oxygen vacancies in the system. Oxygen deficiency plays a significant role in contracting Fe-O bond length in Fe-O₆ octahedra and hence increasing the Fe-O-Fe bond angle in $Bi_{0.9}Ca_{0.1}FeO_{3-\delta}$ and $Bi_{0.9}Pb_{0.1}FeO_{3-\delta}$. The decreased Fe-O bond length and increased Fe-O-Fe bond angle favors the Goodenough-Kanamori-Anderson (GKA) coupling. The GKA coupling increases the magnetic interaction between the spins and hence increases the T_N. Additionally, doping of divalent cations (Ca²⁺ and Pb²⁺) results in the destruction of cycloidal spin structure and formation of a simple antiferromagnetic (AFM) structure. This structure can easily be canted near the heterogeneous interface with a ferromagnetic layer to induce the Dzyaloshinskii-Moriya (DM) interaction and enhance the magneto-electric (M-E) coupling.

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