

Supporting information

Hydrothermal growths, optical features and first-principles calculations of sillenite-type crystals comprising discrete MO_4 tetrahedra

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Fig. S1 Powder X-ray diffraction patterns of M -doped α - Bi_2O_3 crystals ($M = Zn, P, Ni, La, Cd, Cr, Al$) by mild hydrothermal methods.

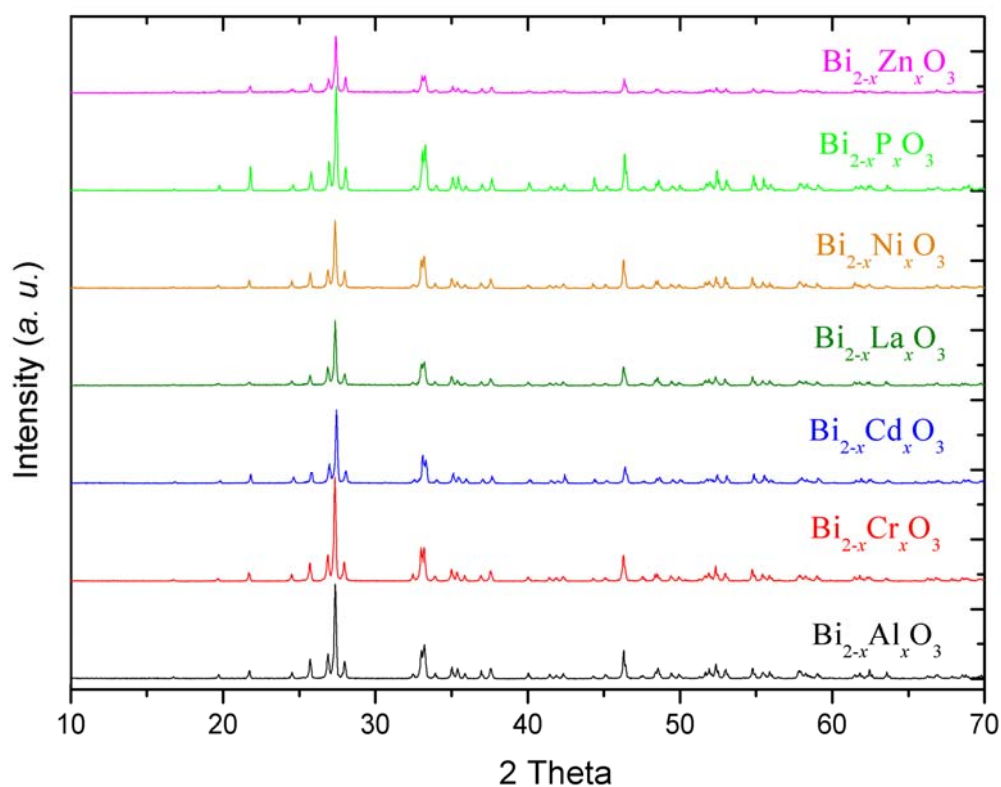


Fig. S2 Unit cell parameters and volumes as a function of the composition of $\text{Bi}_{12}(\text{Bi}_{1-x}\text{Fe}_x)\text{O}_{20}$.

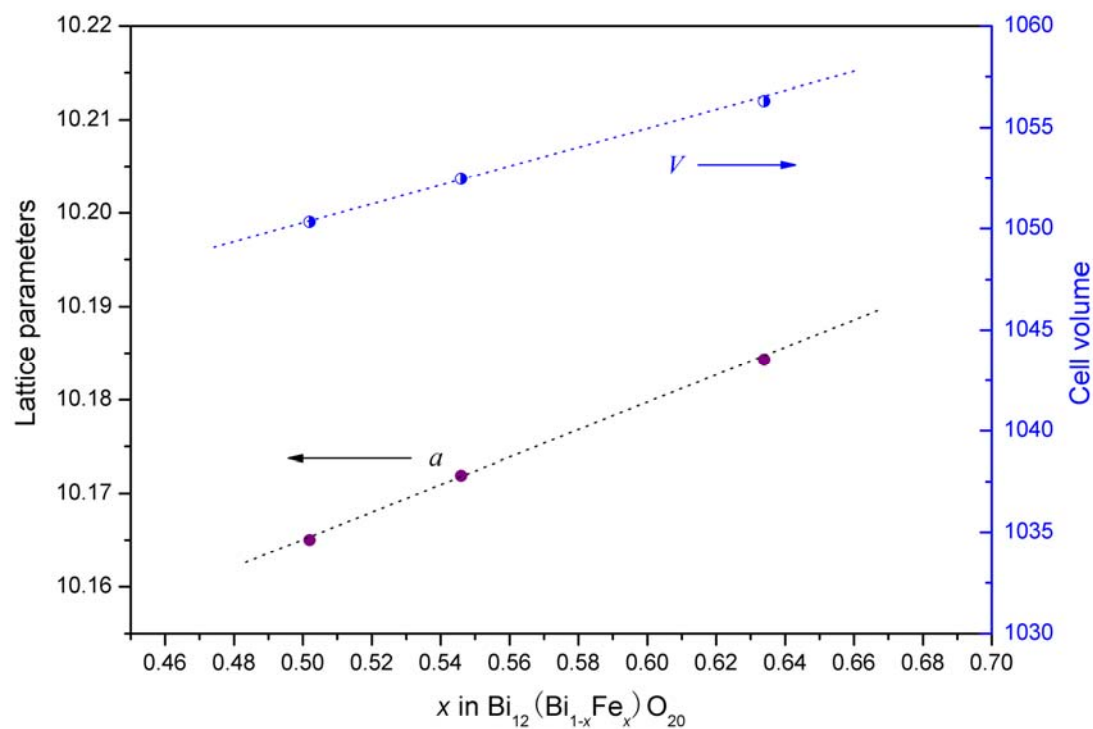
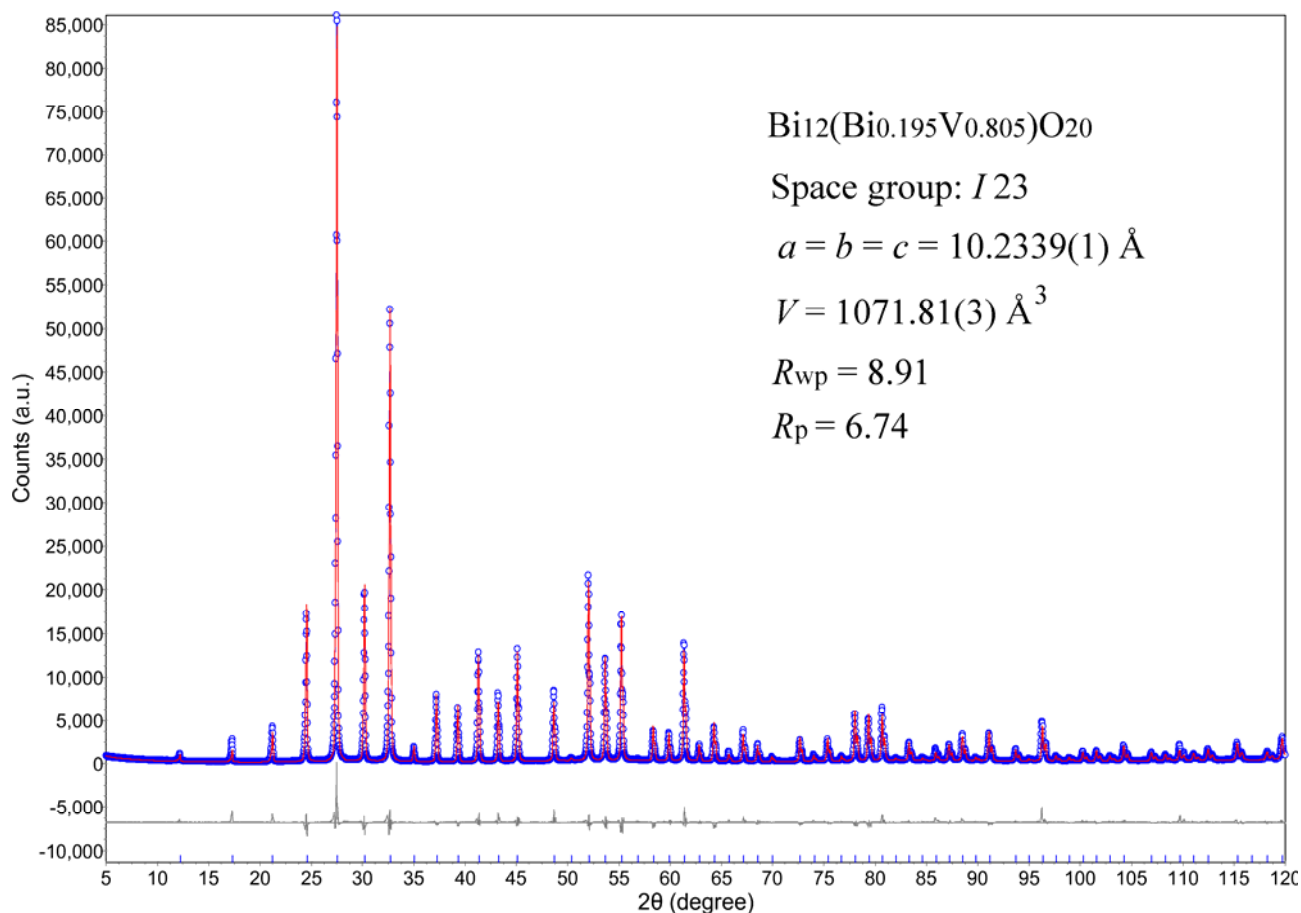
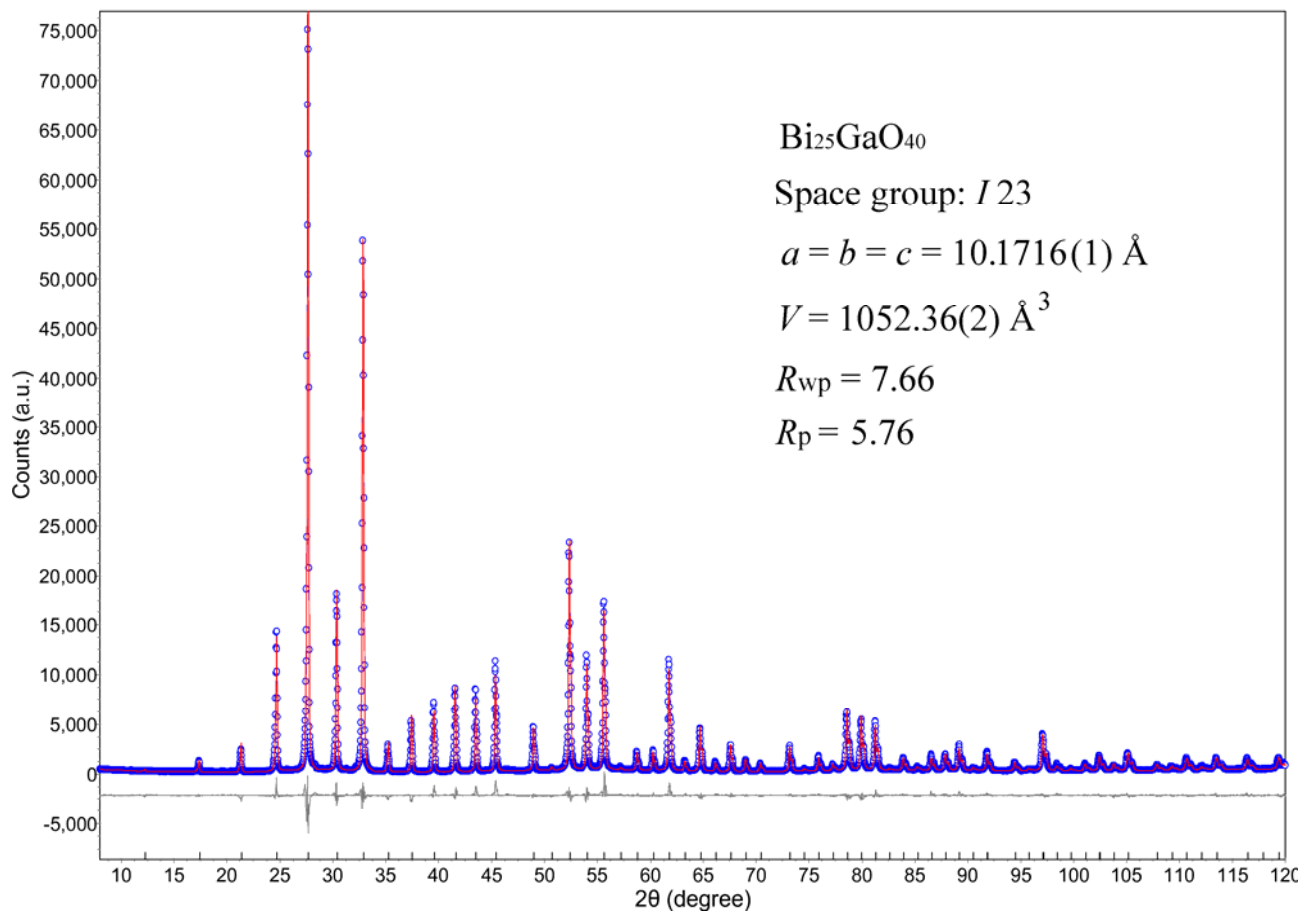
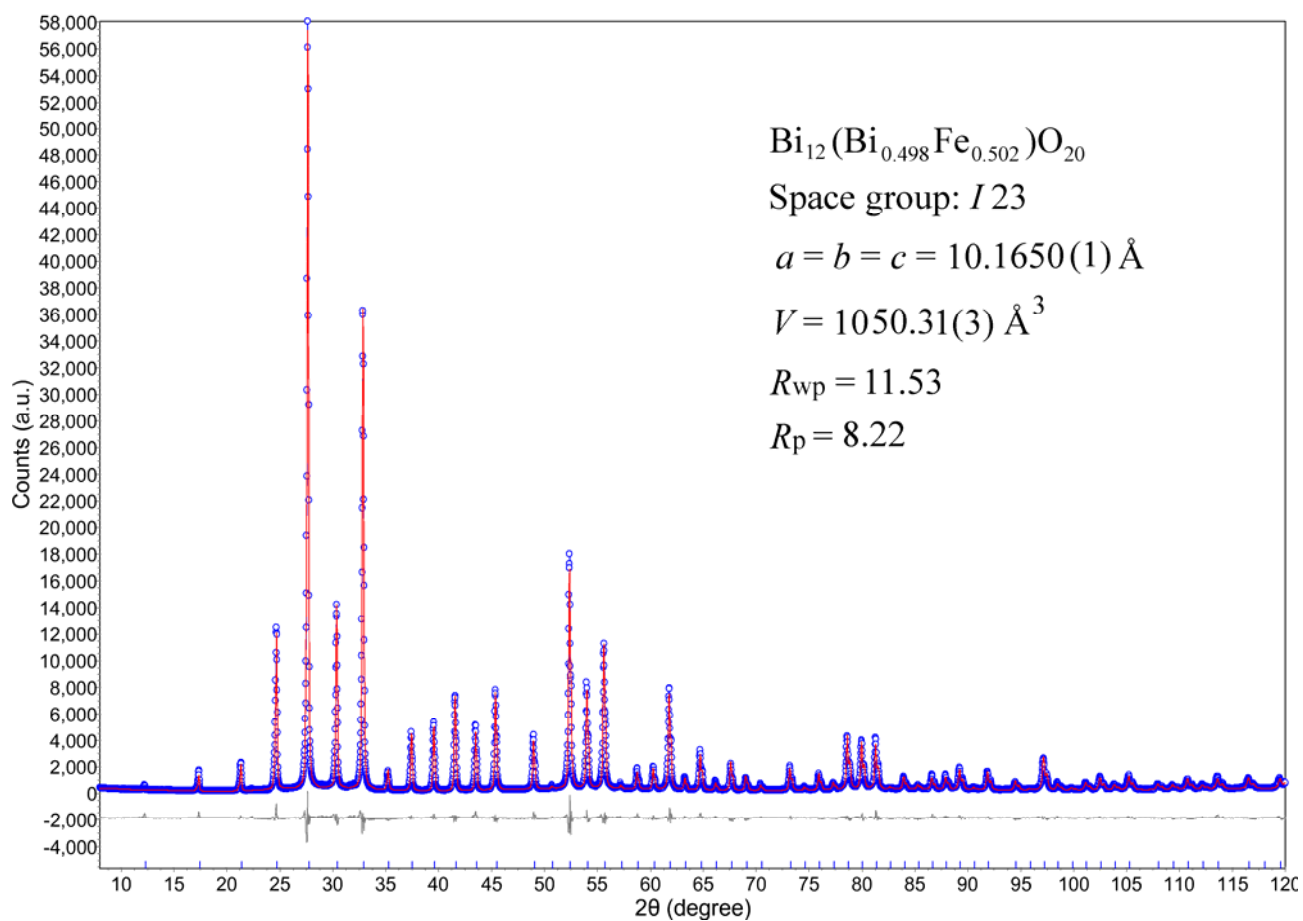
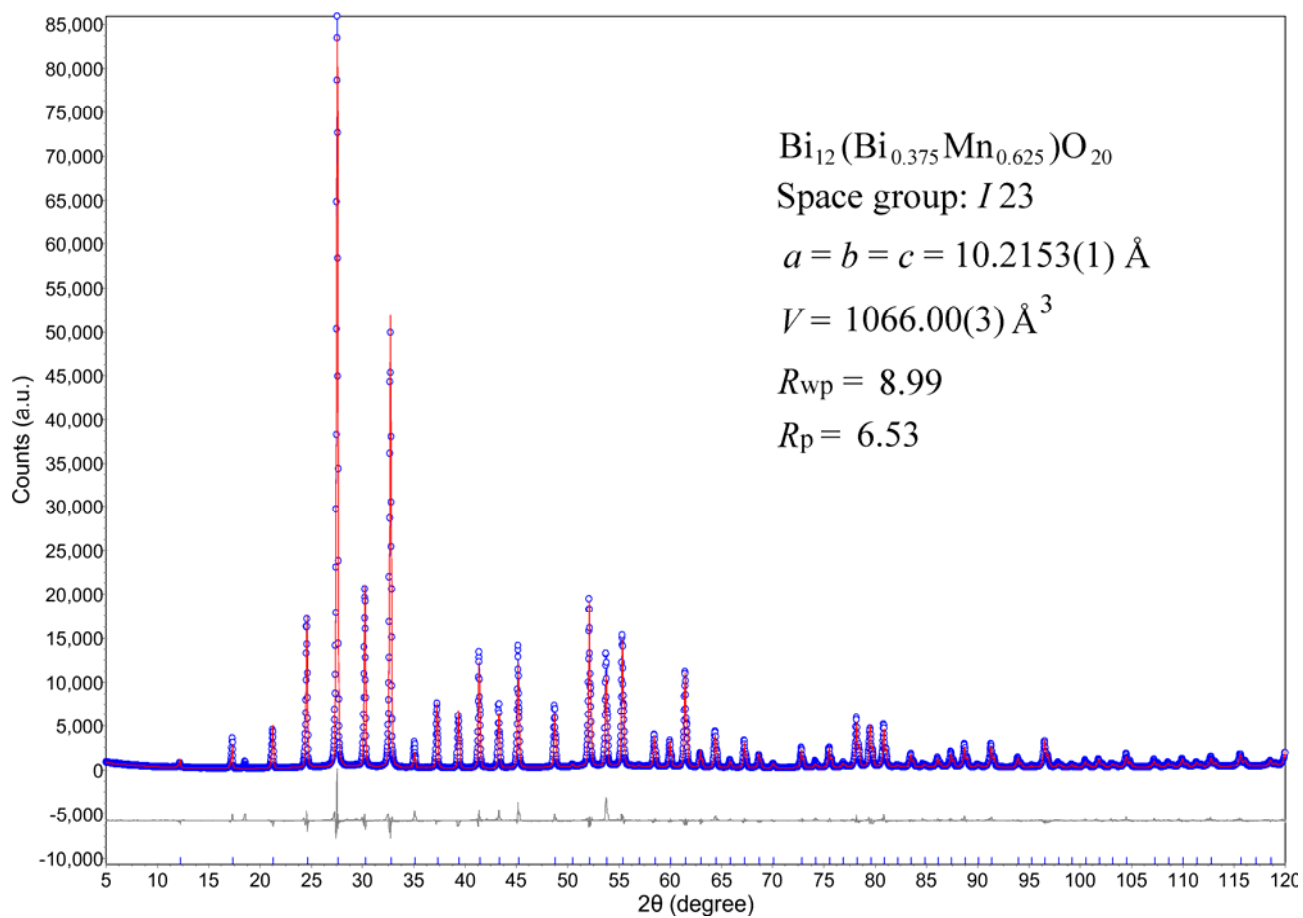
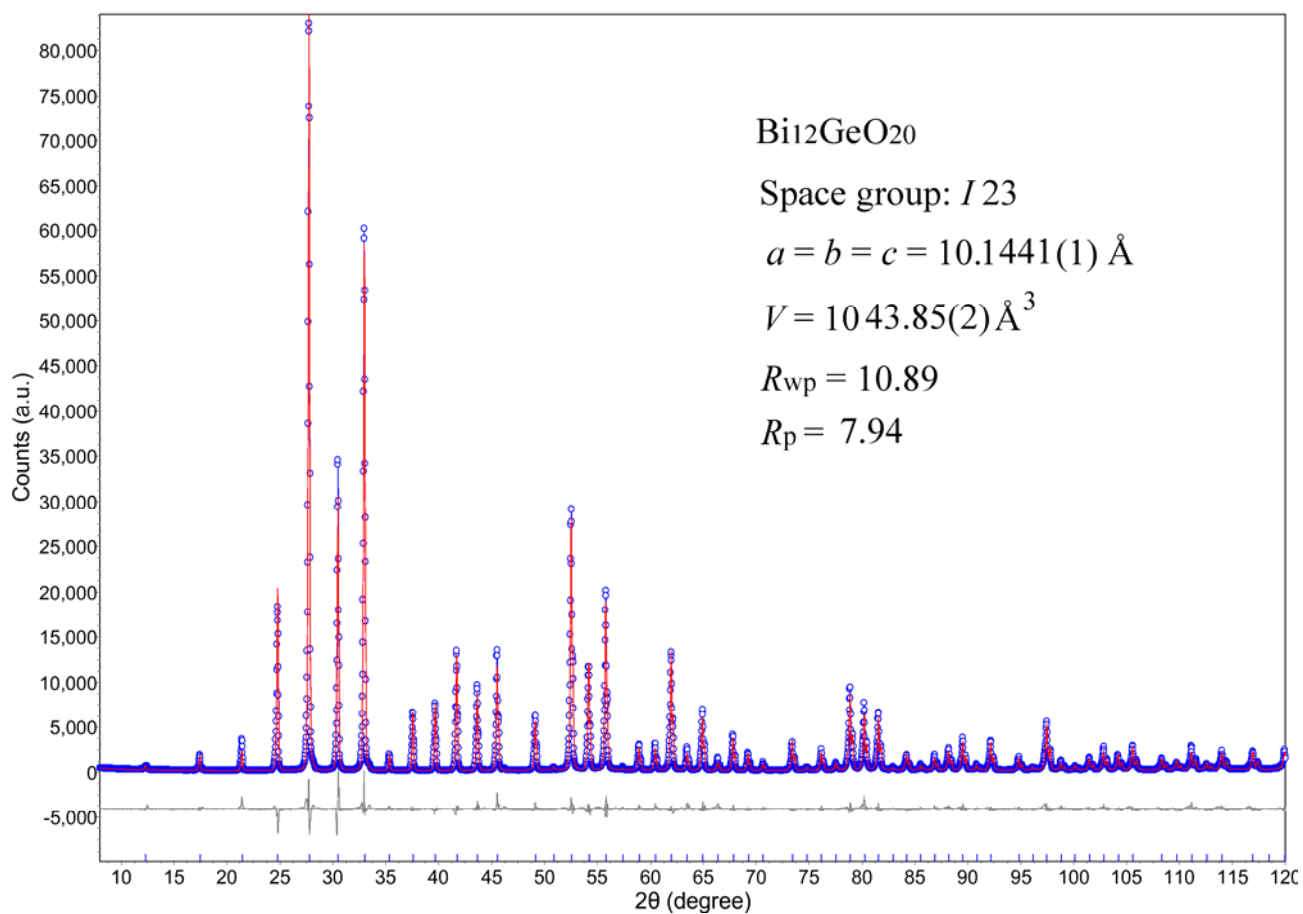


Fig. S3-S8 Rietveld refinement plot of the powder X-ray diffraction profile of $\text{Bi}_{12}(\text{Bi}_x\text{M}_{1-x})\text{O}_{20}$ ($M = \text{V}, \text{Fe}, \text{Ga}, \text{Ge}, \text{Mn}, \text{P}$).







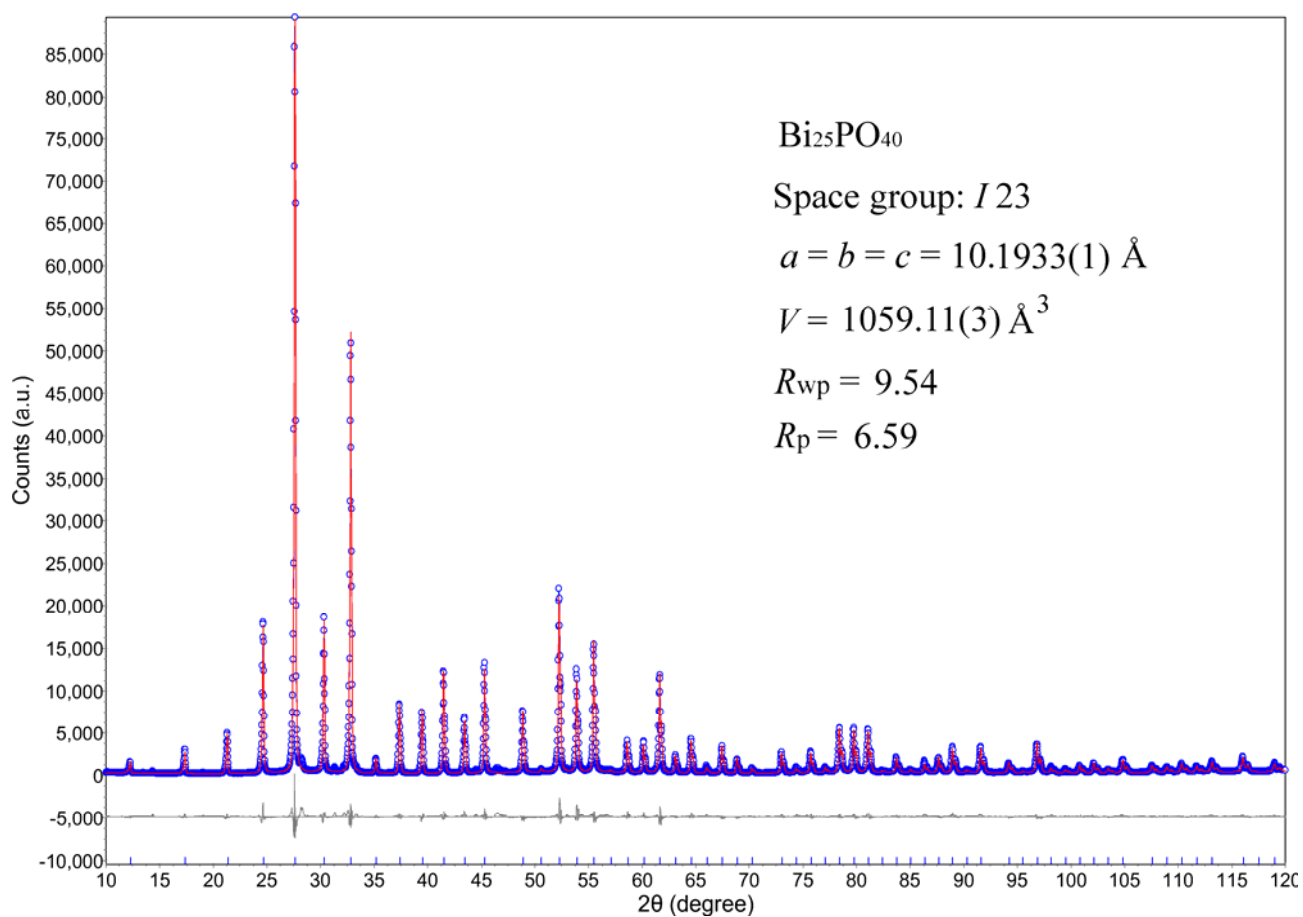


Fig. S9 IR absorbance spectrum of the as-grown $\text{Bi}_{12}(\text{Bi}_{0.375}\text{Mn}_{0.625})\text{O}_{20}$ crystal.

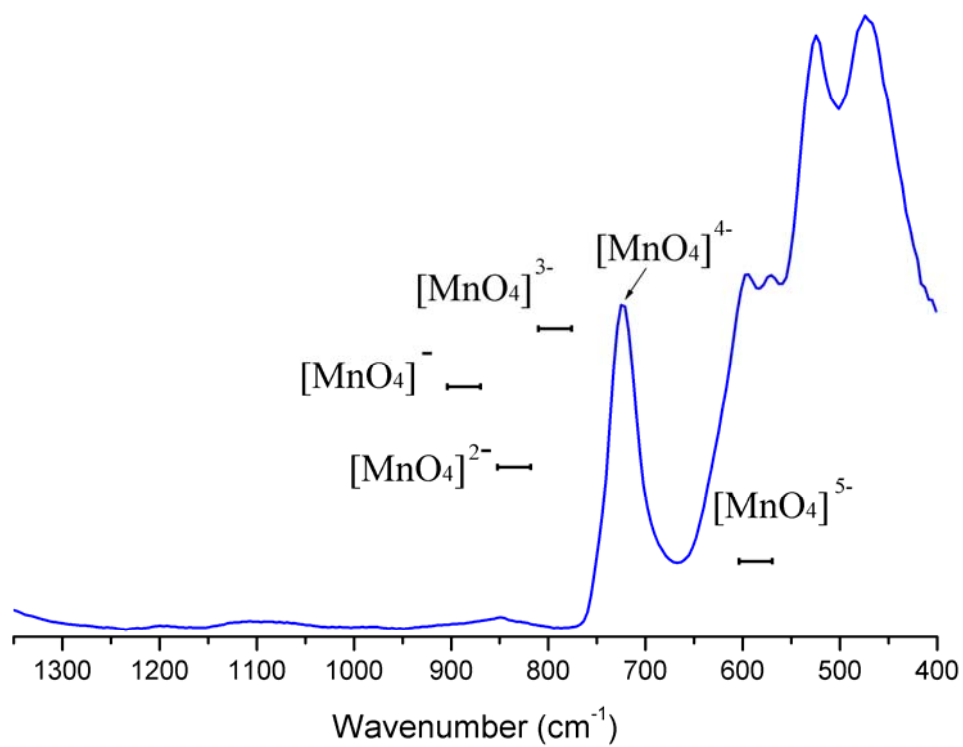


Fig. S10 XPS pattern of the as-grown $\text{Bi}_{12}(\text{Bi}_{0.375}\text{Mn}_{0.625})\text{O}_{20}$ crystal.

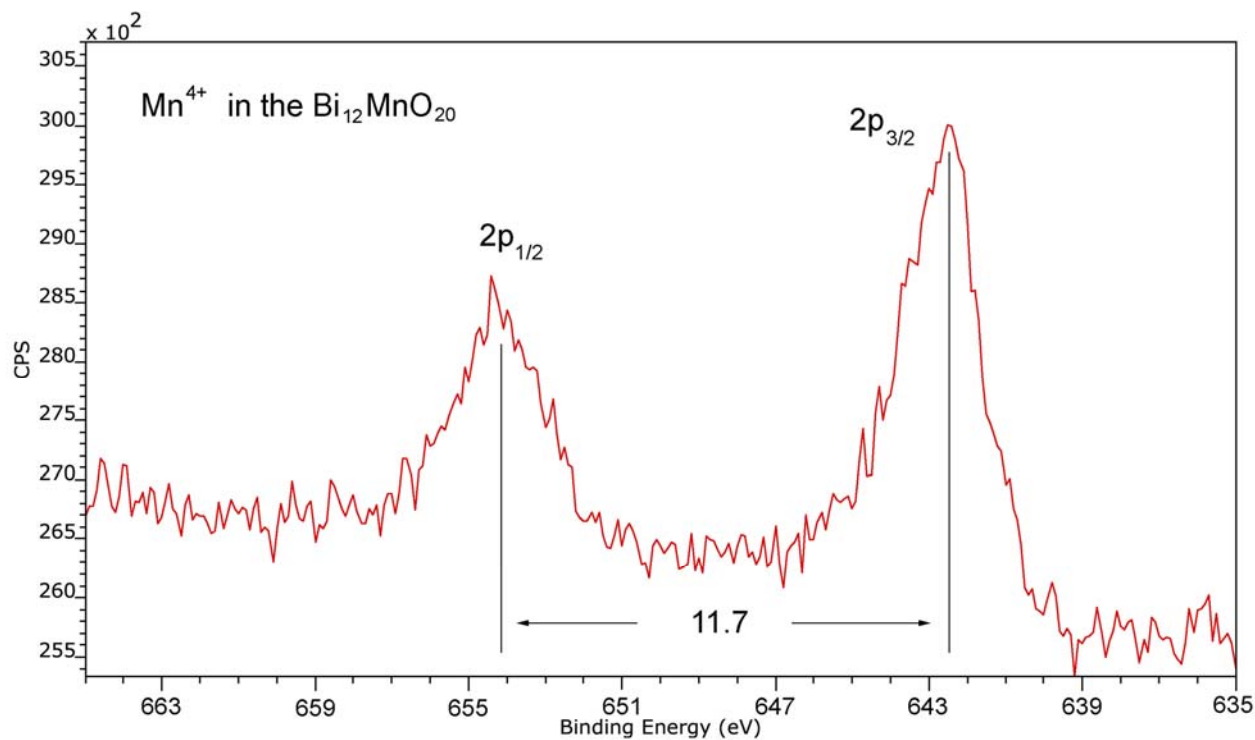


Fig. S11 PDOS projected on each species of atoms in $\text{Bi}_{12}\text{SiO}_{20}$. The straight dashed line indicates the VBM.

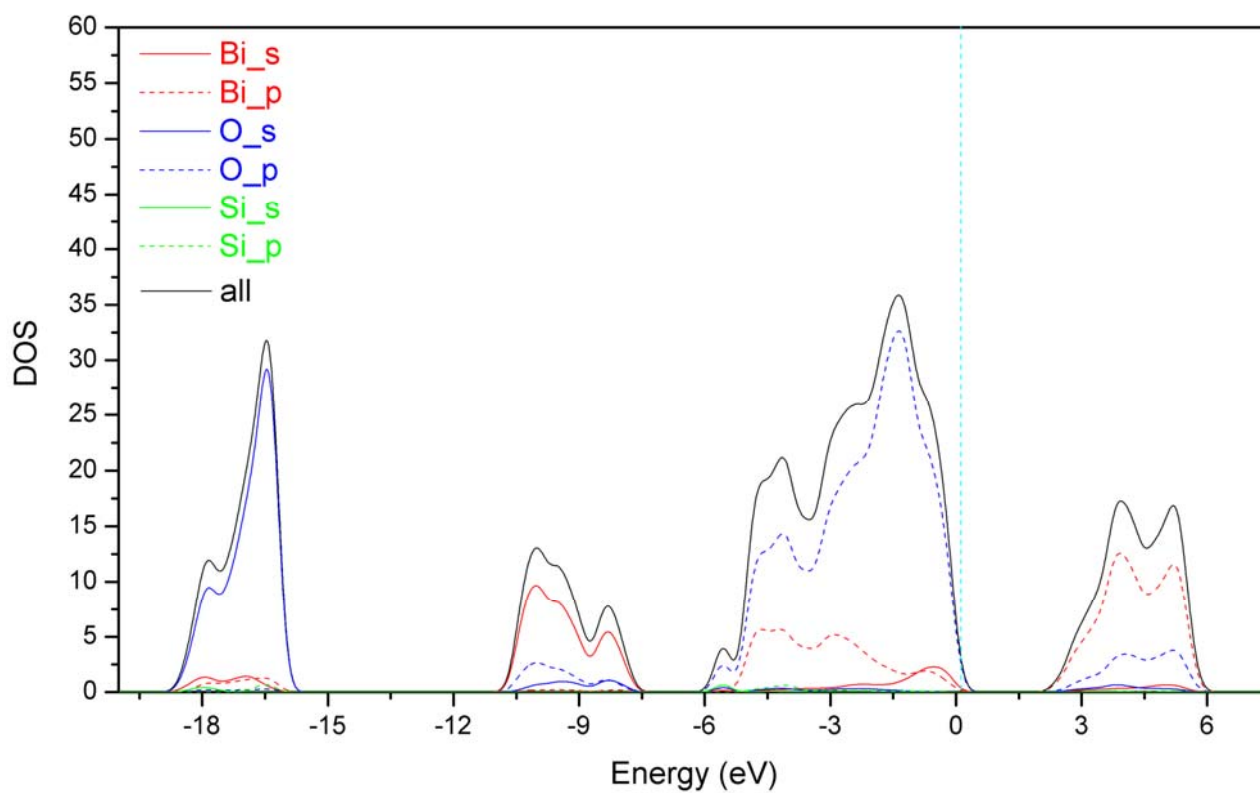


Fig. S12 PDOS projected on each species of atoms in $\text{Bi}_{25}\text{FeO}_{40}$.

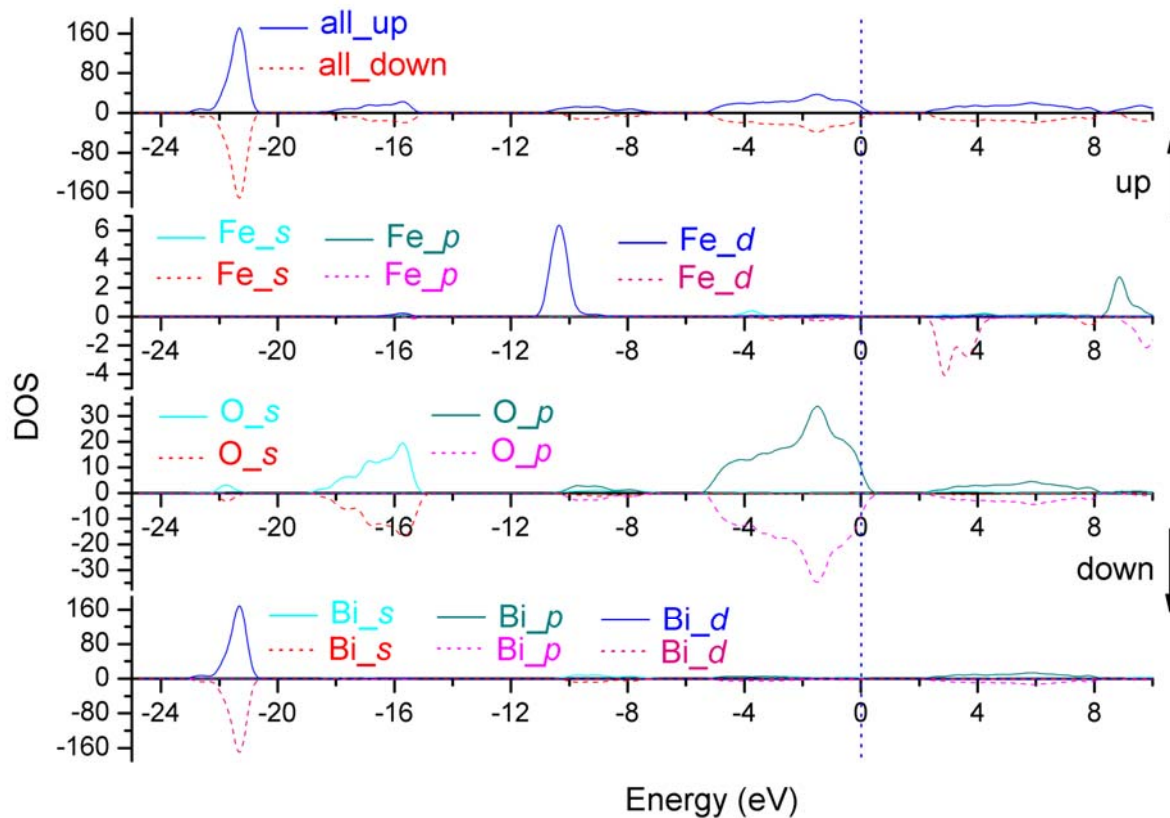


Fig. S13 PDOS projected on each species of atoms in $\text{Bi}_{25}\text{MnO}_{40}$.

