Visible-Light Active Ferroelectric photovoltaics

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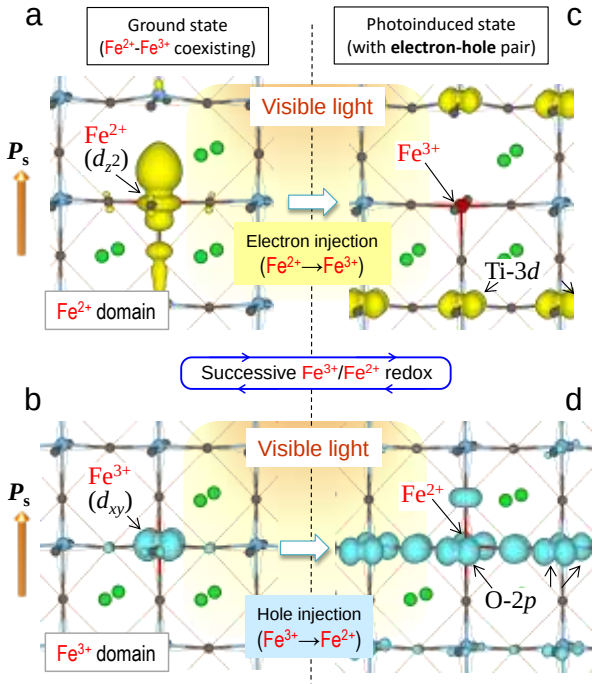


Figure 1 Ground states of ferroelectric Fe-doped $BaTiO_3$ with a spontaneous polarization (P_s) in an Fe^{2+}-Fe^{3+} coexisting state in **a** the Fe^{2+} domain and **b** the Fe^{3+} domain.

Similar to titanium dioxide, a typical photocatalyst, the oxide ferroelectrics suffered from the band-gap problem, namely, photons with energies greater than the bandgap (E_g) can generate electron-hole pairs that deliver the robust PV effect. Our group reported the gap-state engineering[1] that mid-gap states act as a scaffold for visible-light activation of the PV response in $BiFeO_3$. However, this materials design was still restricted by the materials E_g, i.e., the photon energies greater than the half of E_g was required for generating electron-hole pairs.

The motivation of our study was quite simple; how transition metal cations that can have multiple valence states influence the PV effects. We chose Mn-doped $BiFeO_3$[1–4] and iron doped barium titanate (Fe-$BaTiO_3$)[5]. At first, we anticipated that a higher concentration of Fe^{2+} that creates a donor state induce larger photocurrents. The experimental results were qualitatively consistent with this expectation, but the reduced sample exhibited extraordinary large photocurrents. This result cannot be explained solely by the role of Fe^{2+}. The subsequent experimental and theoretical investigations revealed that the coexisting of Fe^{3+} and Fe^{2+} provided the robust PV effect. As shown in Fig. 1, the Fe^{2+}-Fe^{3+} coexisting state, namely the polar lattice with the Fe^{2+} and Fe^{3+} domains having the donor and acceptor states, respectively, undergoes electron and hole injections under light illumination. Visible light with energies much smaller than E_g can, in principle, induces electron-hole pair generation, which is accompanied by the redox reactions of iron both in the domains.

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Hiroki Matsuo received a bachelor's degree, an M.S degree, and a Ph.D. degree in Applied Chemistry from University of Tokyo, Japan. He is a Research Associate of IROAST of Kumamoto University, Japan. He has his expertise in thin-film fabrication by pulsed laser deposition of functional materials including dielectric and ferroelectric perovskite oxides.

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Notes/Comments