Supplementary Information

Atomic Doping to Enhance the p-type Behavior of $BiFeO_3$ Photoelectrodes for Solar H_2O_2 Production

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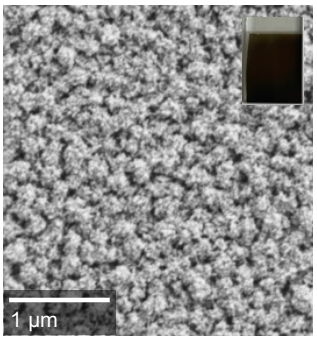

Fig. S1 An SEM image of an as-deposited Bi/Fe film. The inset shows a photograph of the corresponding film.

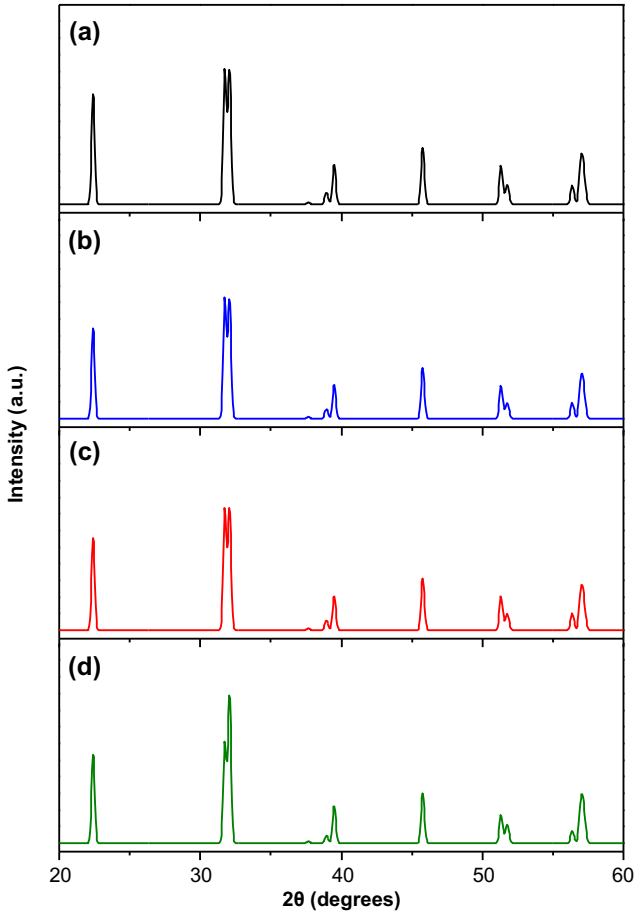

Fig. S2 Simulated XRD patterns for (a) pristine $BiFeO_3$ (ICSD #51664) with no preferential orientation, (b) $Bi_{0.93}FeO_3$ with no preferential orientation, (c) $Na_{0.07}Bi_{0.93}FeO_3$ with no preferential orientation and (d) $Na_{0.07}Bi_{0.93}FeO_3$ with (110) preferential orientation.

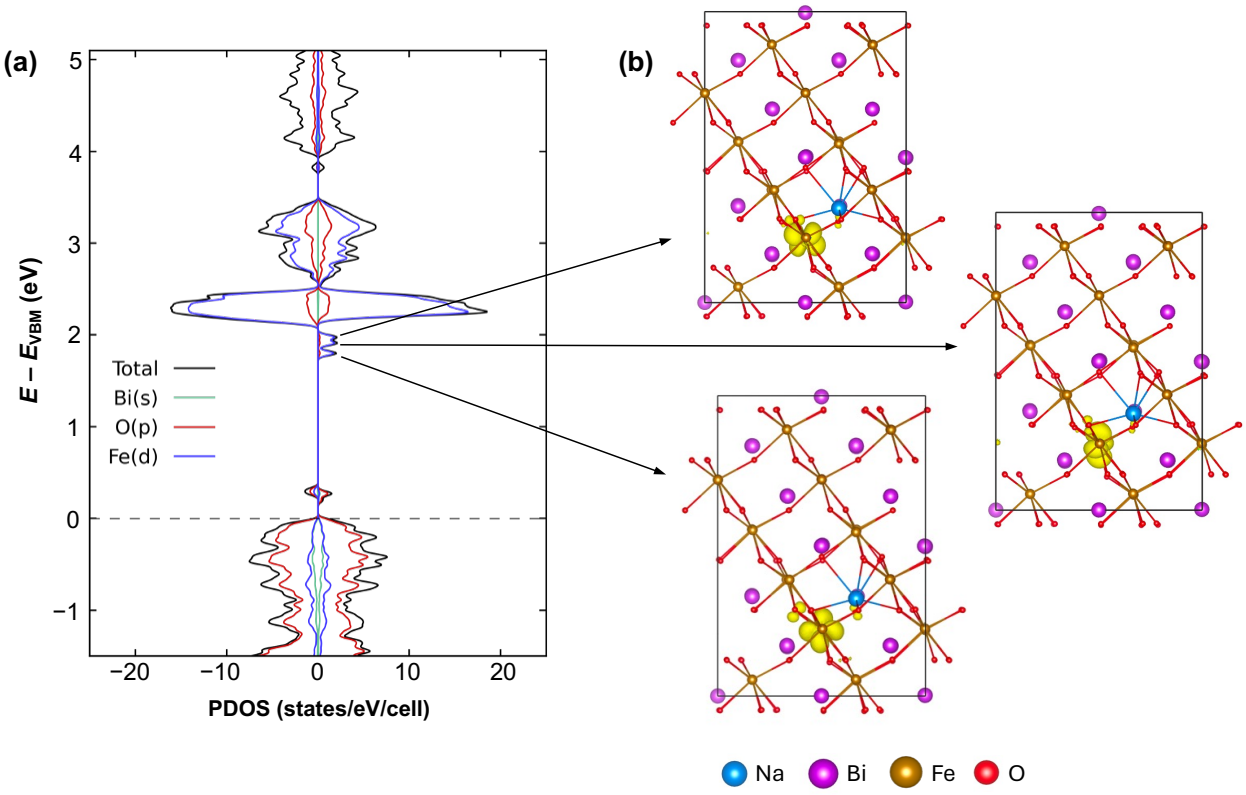

Fig. S3 $BiFeO_3$ with a single Na substituted on Bi in a 120-atom supercell. (a) Projected density of states (PDOS) with spin up having positive values and spin down having negative values. (b) The norm-squared wavefunctions of the perturbed conduction band states right below the conduction band showing the character of t_{2g} of Fe atoms. The isosurface value is 1% of the maximum amplitude of the wavefunction.

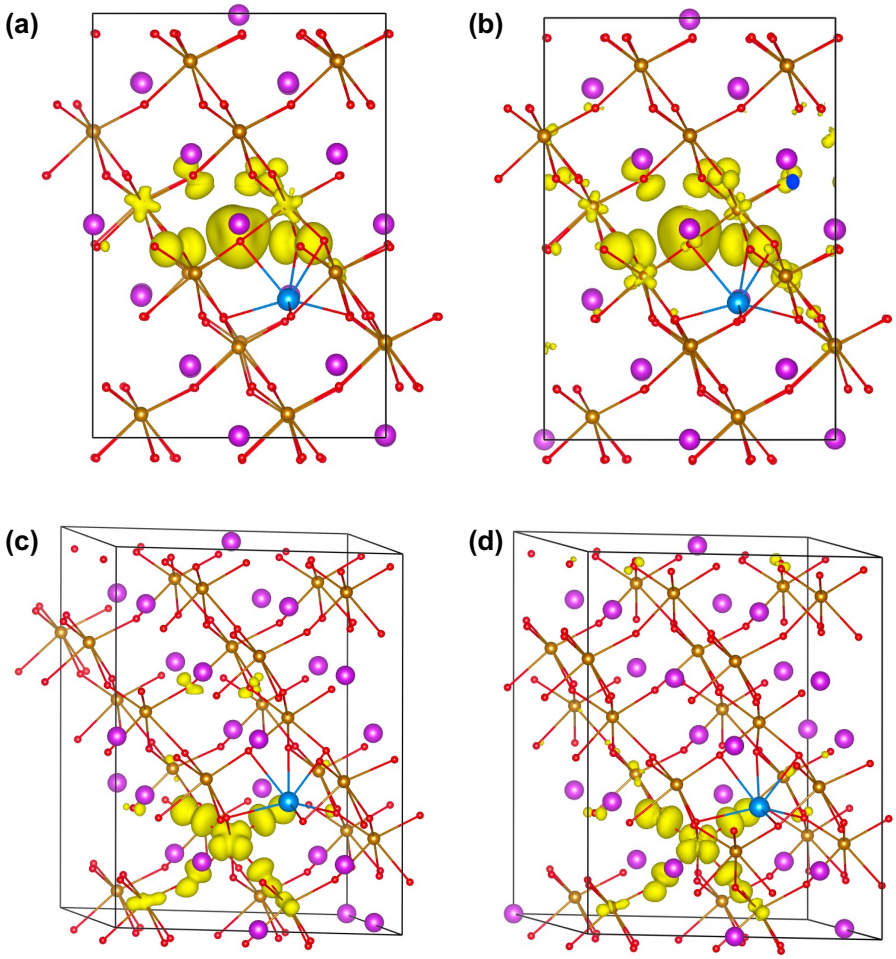

Fig. S4 Norm-squared wave functions of the two hole-polarons computed using functionals HSE06 (**a** and **c** for spin up and spin down, respectively) and PBE+U (**b** and **d** for spin up and spin down, respectively). The isosurface value is 1% of the maximum amplitude of the wavefunction.

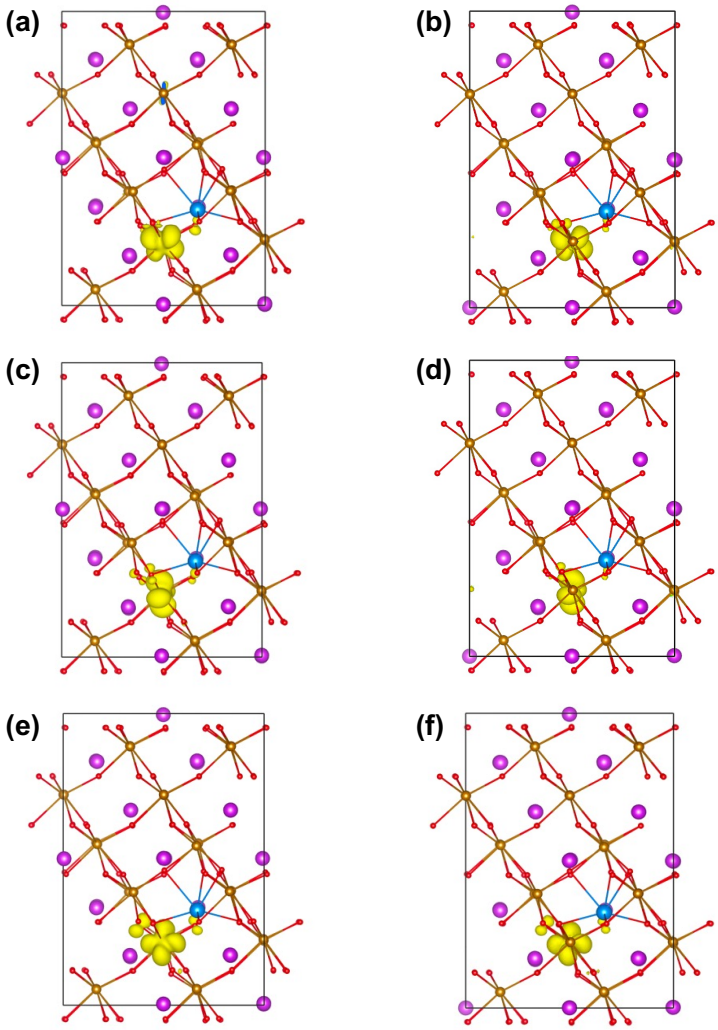

Fig. S5 Norm-squared wave functions of the perturbed conduction band states below the CBM computed using functionals HSE06 (**a**, **c**, and **e**) and PBE+U (**b**, **d**, and **f**). The isosurface value is 1% of the maximum amplitude of the wavefunction.