

Supporting Information

n-type Doping of BiVO₄ by Different F-doped Concentrations for Improving the Electronic Character of BiVO₄ as Photoanode Nanomaterial for Solar Water Splitting: A First-principles Study

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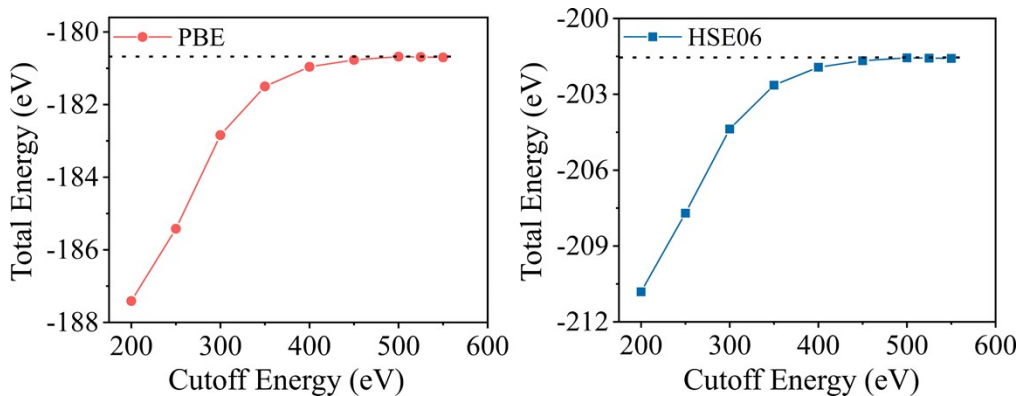


Figure S1. Convergence test results with respect to kinetic-energy cutoff.

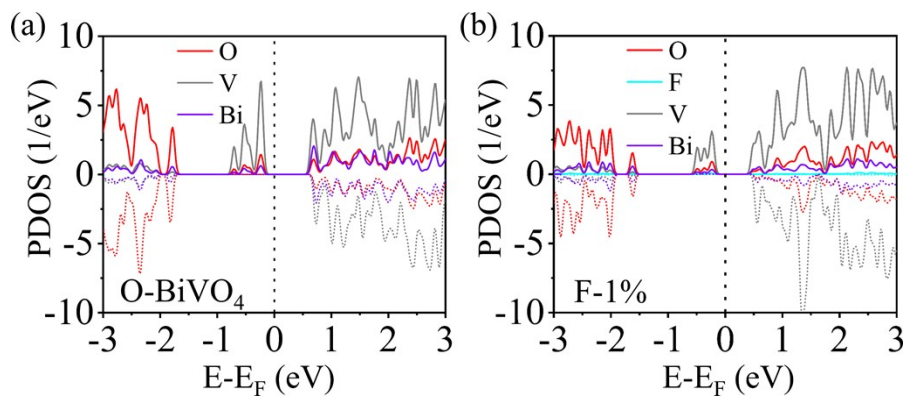


Figure S2. Projected density of states of (a) O-BiVO₄ (one O atom vacancy) and (b) F-doped BiVO₄ (replacing one O atom with F atom) obtained at the HSE06 level.

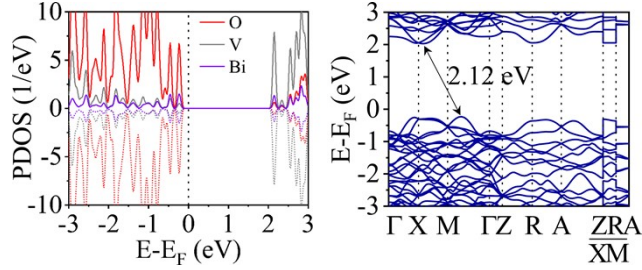


Figure S3. projected density of states and electronic band structure of pristine BiVO_4 crystal calculated by the PBE function.

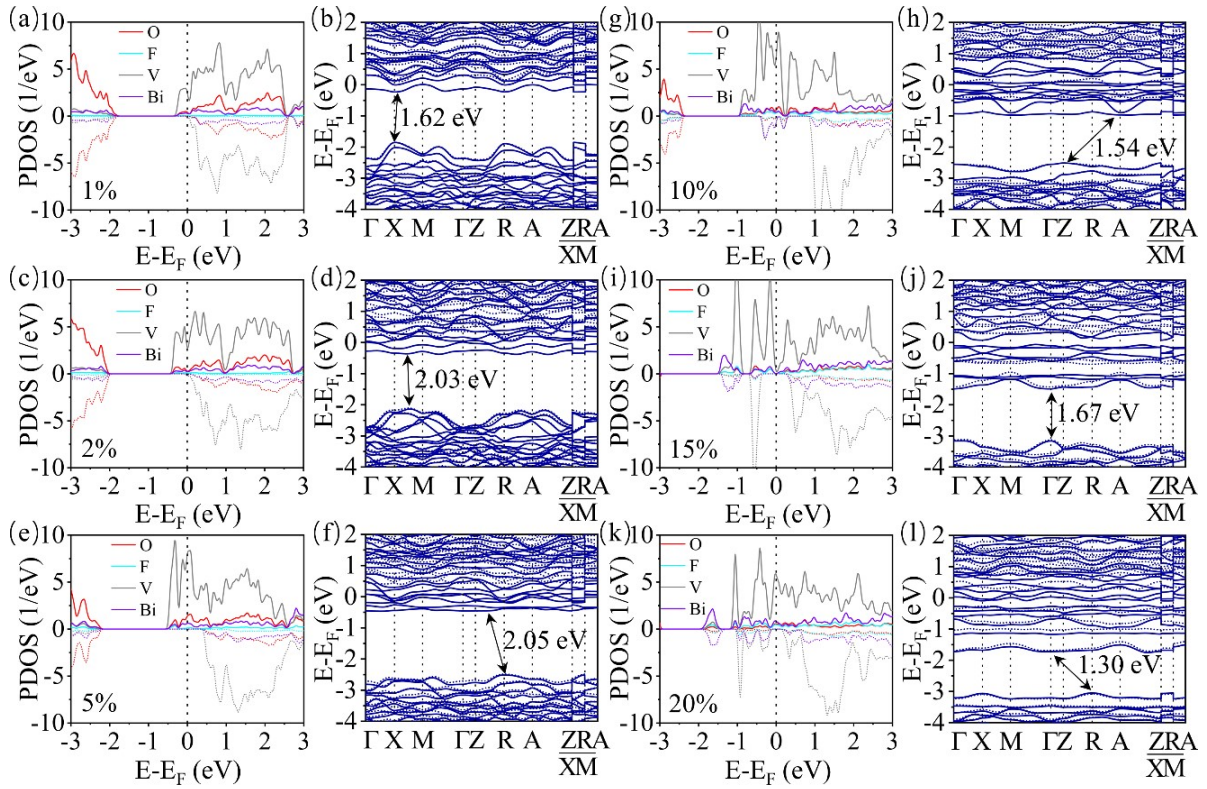


Figure S4. Projected density of states and electronic band structures of F-doped BiVO_4 crystal with different doping mass concentrations calculated by the PBE function. The solid and dash lines represent projections to the spin-up, spin-down states of the F-doped BiVO_4 , respectively, and the VBM and CBM are indicated by the black arrows.

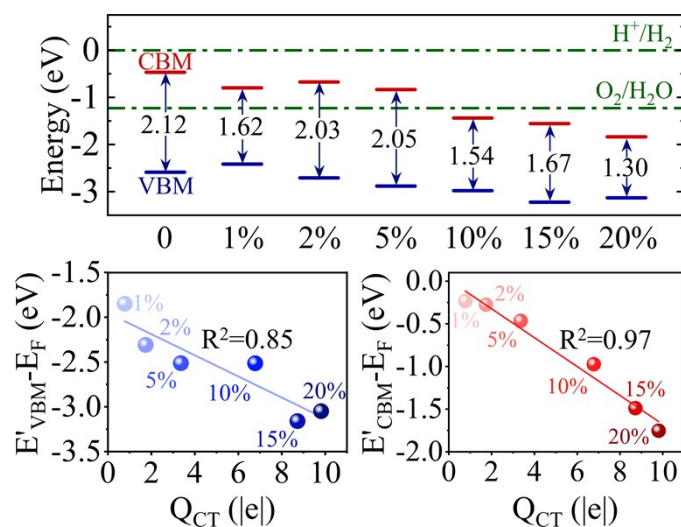


Figure S5. Top panel: calculated band gaps and band edge positions of pristine and F-doped $BiVO_4$ at the PBE level, which are given relative to the standard redox potentials for water splitting. Bottom panels: linear relationship between the frontier energy level shift (relative to the Fermi level) and the total charge transfer amounts from doping F atoms to other atoms involved in F-doped $BiVO_4$ (bottom panel).