Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information for

Tuning band gaps and optical absorption of BiOCl through doping and strain：Insight form DFT calculations

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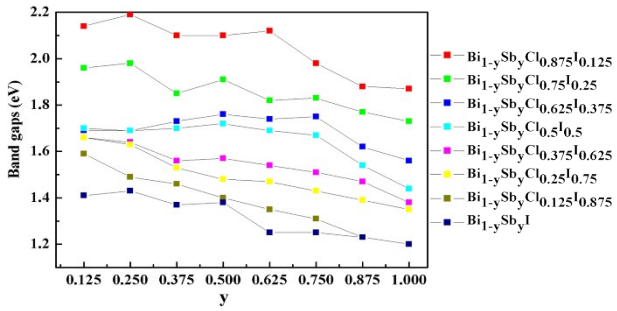

Figure S1. The band gaps of $Bi_{1-y}Sb_yOCl_{0.875}I_{0.125}$, $Bi_{1-y}Sb_yOCl_{0.75}I_{0.25}$, $Bi_{1-y}Sb_yOCl_{0.625}I_{0.375}$, $Bi_{1-y}Sb_yOCl_{0.5}I_{0.5}$, $Bi_{1-y}Sb_yOCl_{0.375}I_{0.625}$, $Bi_{1-y}Sb_yOCl_{0.25}I_{0.75}$, $Bi_{1-y}Sb_yOCl_{0.125}I_{0.875}$, $Bi_{1-y}Sb_yOI$ which were shown in red, green, blue, cyan, magenta, yellow, daek yellow and royal respectively.

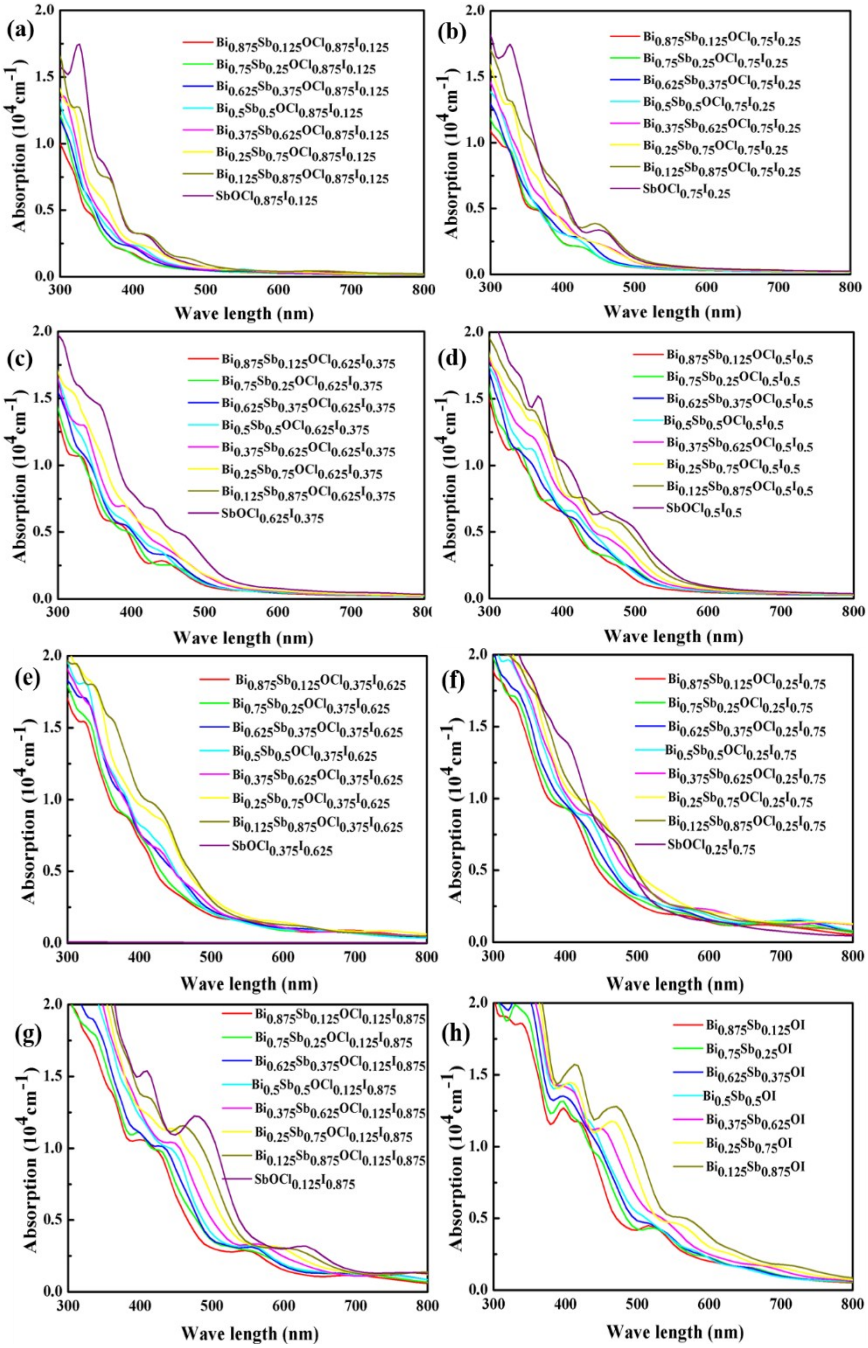

Figure S2. The absorption coefficients of $Bi_{1-y}Sb_yOCl_{0.875}I_{0.125}$, $Bi_{1-y}Sb_yOCl_{0.75}I_{0.25}$, $Bi_{1-y}Sb_yOCl_{0.625}I_{0.375}$, $Bi_{1-y}Sb_yOCl_{0.5}I_{0.5}$, $Bi_{1-y}Sb_yOCl_{0.375}I_{0.625}$, $Bi_{1-y}Sb_yOCl_{0.25}I_{0.75}$, $Bi_{1-y}Sb_yOCl_{0.125}I_{0.875}$, $Bi_{1-y}Sb_yOI$ which were shown in (a), (b), (c), (d), (e), (f), (g) and (h) respectively.

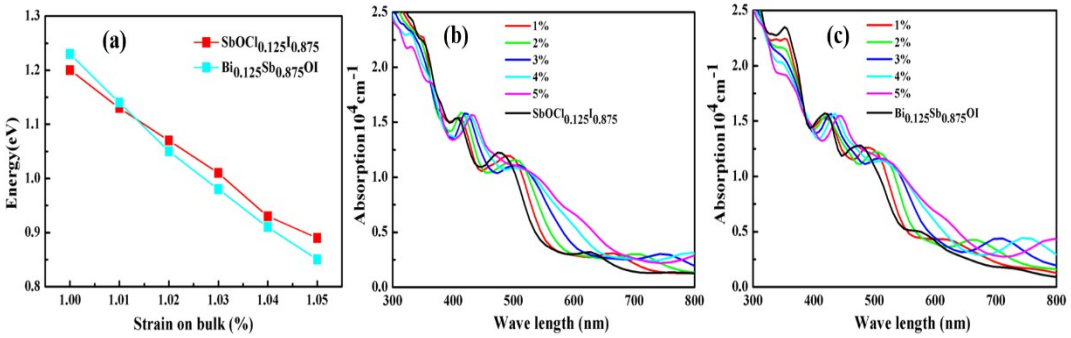

Figure S3. Calculated band gaps of tensile strained $SbOCl_{0.125}I_{0.875}$ and $Bi_{0.125}Sb_{0.875}OI$ (a), and corresponding absorption coefficients (b) and (c).

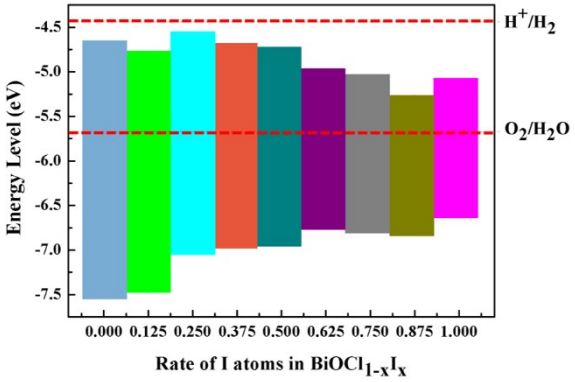

Figure S4. Band edge positions of $BiOCl_{1-x}I_x$. The energy scale is shown in the normal hydrogen electrode and the redox potential of water splitting are shown in red dot line.

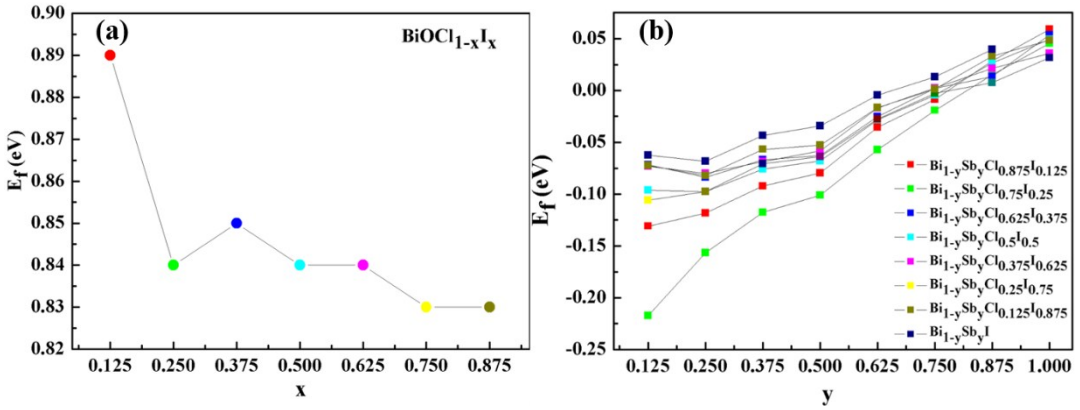

Figure S5. Formation energy of $BiOCl_{1-x}I_x$ and $Bi_{1-y}Sb_yOCl_{1-x}I_x$ are shown in (a) and (b) respectively.