Supporting Information

Ti-alloying of BaZrS$_3$ chalcogenide perovskite for photovoltaics

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Figure S1. (a) The XRD patterns of Ba(Zr$_{1-x}$Ti$_x$)O$_3$ powder samples for $x=0$, 0.01, 0.02, 0.03, and 0.04. All peaks shift to higher angles, and the amount of shift increases with increasing $x$. The inset is an enlarged view of (110) peak. The maximum peak shift for 4% alloyed sample is 0.11° (shown by the two dotted lines); (b) The XRD pattern of Ba(Zr$_{1-x}$Ti$_x$)O$_3$ powders for $x=0$, 0.05, 0.075, and 0.1. The inset is an enlarged view of (110) peak. The maximum peak shift for the 10% alloyed sample is 0.19° (shown by the two dotted lines).
Figure S2. The typical SEM images of (a) 0 at%, (b) 1 at%, (c) 2 at%, (d) 3 at%, (e) 4 at%, (f) 5 at%, (g) 7.5 at%, and (h) 10 at% Ti alloyed Ba(Zr$_{1-x}$Ti$_x$)$_3$ powder samples. All scale bars are 5 µm.
Figure S3. (a) The XRD patterns of Ba(Zr$_{1-x}$Ti$_x$)S$_3$ for $x$=0, 0.05, 0.075, and 0.1. The additional peaks indicated by vertical black lines from left to right are assigned to BaS (110), BaTiS$_3$ (201), BaS (111), ZrO$_2$ (220), TiS$_2$ (110), and ZrS$_2$ (201) peaks, respectively; The enlarged view of (b) (121) peak; (c) (040) peak; and (d) (240) peak of BaZr$_3$S$_3$, showing peaks shifting to higher angles as Ti alloying percentage increases.
Figure S4. The Raman spectra of Ba(Zr_{1-x}Ti_x)S_3 for x=4, 7.5, and 10 at%, measured at room temperature. More Raman scattering modes appear, indicating phase separation at higher Ti alloying concentrations. Peaks labeled with asterisk marks (370 cm\(^{-1}\) and 473 cm\(^{-1}\)) cannot be assigned to BaZrS\(_3\) phase, which may be from BaTiS\(_3\) or binary phases.
Figure S5. The Tauc plot of Ba(Zr$_{1-x}$Ti$_x$)S$_3$ powders for x=0, 0.075, and 0.1. Tails in the absorption spectra at lower energies come from secondary phases for 7.5 and 10 at% Ti alloyed samples.