

**Supporting Information for**  
**“Screening novel candidates for mid-IR nonlinear optical**  
**materials from I<sub>3</sub>-V-VI<sub>4</sub> compounds”**

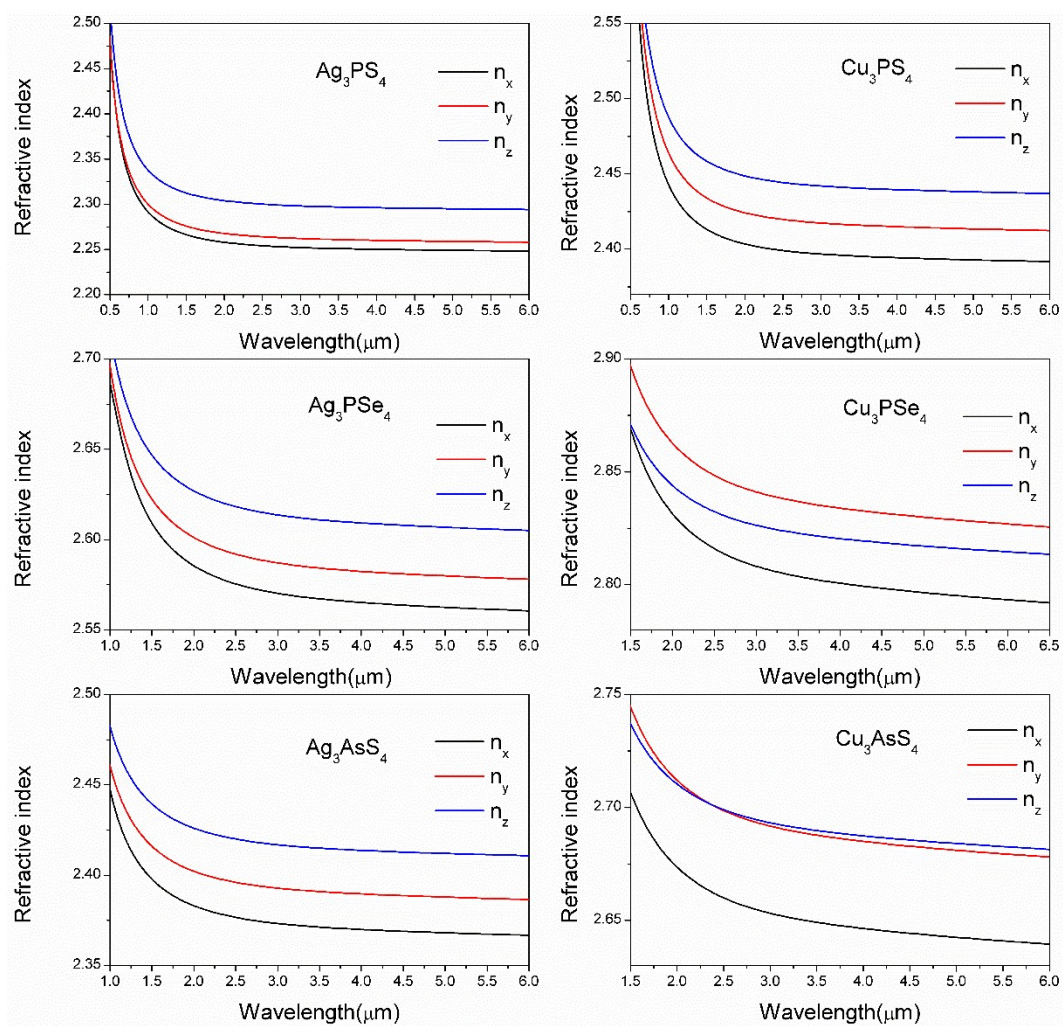
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**Figure S1.** The calculated dispersion curves of refractive indices in  $\text{I}_3\text{-V-VI}_4$  compounds (with  $\text{I} = \text{Ag}$  or  $\text{Cu}$ ,  $\text{V} = \text{P}$  or  $\text{As}$ , and  $\text{VI} = \text{S}$  or  $\text{Se}$ ) by the hybrid HSE06 functional.