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Design of I_2-II-IV-VI_4 Semiconductors through Element-substitution: the Thermodynamic Stability Limit and Chemical Trend SHIYOU CHEN, East China Normal University, CONGCONG WANG, Fudan University, HONGJUN XIANG, XIN-GAO GONG, Fudan University, ARON WALSH, University of Bath, SU-HUAI WEI, National Renewable Energy Laboratory — Through element substitution in kesterite Cu_2ZnSnS_4 or $Cu_2ZnSnSe_4$, a class of I_2-II-IV-VI_4 semiconductors can be designed as novel functional materials. Using the first-principles calculations, we show that this element-substitution design is thermodynamically limited, i.e., although I_2-II-IV-VI_4 with I=Cu, Ag, II=Zn, Cd, Hg, IV=Si, Ge, Sn and VI=S, Se, Te are stable quaternary compounds, those with II=Mg, Ca, Sr, Ba, IV =Ti, Zr, Hf, and VI=O are unstable against the phase-separation into the competing binary and ternary compounds. Three main phase-separation pathways are revealed. In general, we show that if the secondary II-VI or I_2-IV-VI_3 phases prefer to have non-tetrahedral structures, then the I_2-II-IV-VI_4 semiconductors tend to phase separate. This finding can be used as a guideline for future design of new quaternary semiconductors.

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