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Engineering Group-IV Monochalcogenides by Doping and Alloying HANSIKA SIRIKUMARA, TREVOR FITZPATRICK, THUSHARI JAYASEKERA, Southern IL Univ-Carbondale — Group-IV monochalcogenides, MX (M=Sn,Ge and X=S,Se) have shown to be promising materials for thermoelectric and photovoltaic applications. These properties can be further engineered by substitutional doping and alloying. Using the results from ab initio Density Functional Theory calculations, we identified a series of new class of monochalcogenide alloys in the form Ge(1-x)SnxS, Ge(1-x)SnxSe, GeSxSe(1- x), SnSxSe(1-x). Stability of their two-dimensional counterparts will also be discussed in this presentation.

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