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Tin sulfides and tin selenides at ambient and high pressure conditions KIEN NGUYEN CONG, JOSEPH GONZALEZ, BRAD STEELE, IVAN OLEYNIK, University of South Florida — The application of high pressure promotes unusual chemical bonding in condensed phase resulting in the synthesis of novel materials, which may be recoverable in metastable states at ambient conditions. First-principles evolutionary crystal structure search is performed to explore novel tin sulfide (Sn_xS_y) and tin selenide (Sn_xS_y) crystals with the goal to discover novel photovoltaic and thermoelectric materials. Variable stoichiometry searches at various pressures are performed and the phase diagrams are constructed in the range of pressures 0-100 GPa, which include both the thermodynamically stable and lowest enthalpy metastable structures. Several new structures are identified and their dynamical stability is investigated. To help experimental synthesis of these novel compounds, Raman spectra and XRD patterns are also calculated. These new materials are also investigated to identify those with promising photovoltaic and thermoelectric properties.

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