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Band structure investigations of $SnZrCh_3$ (Ch=S and Se) by DFT and XPS ANNETTE RICHARD, Department of Chemistry, Oregon State University, DANIEL HARADA, ANDRIY ZAKUTAYEV, ROBERT KYKYNESHI, JANET TATE, Department of Physics, Oregon State University, ANDREAS KLEIN, Division of Surface Science, Darmstadt University of Technology — $SnZrS_3$, a p-type semiconductor with a measured band gap of 1.5 eV, is a possible material for a solar cell absorber layer. We report the theoretical investigations into this layered compound structure. Preliminary results show that $SnZrS_3$ is p-type semiconductor with an estimated indirect band gap of 0.73eV. The valence band is constructed from sulfur p and tin s-orbitals. Theoretical results are compared to x-ray photoelectron spectroscopy measurements. Correlations to the binary compounds $ZrCh_2$ and SnCh will be made and the effects of p-type and $n-$type doping in $SnZrCh_3$ (Ch= S, Se) will be discussed.

Annette Richard
Department of Chemistry, Oregon State University

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