Pressure and Temperature Dependent Raman Spectroscopy of Chalcogenide Perovskites
NELSON GROSS, SAMANTHE PERERA, XIUCHENG WEI, State University of New York at Buffalo, YIYANG SUN, None, SHENGBAI ZHANG, Rensselaer Polytechnic Institute, HAO ZENG, B. A. WEINSTEIN, State University of New York at Buffalo — Inorganic semiconductors known as chalcogenide perovskites including BaZrS$_3$ and its alloys, show potential for application in photovoltaics. The phonon frequencies of BaZrS$_3$ have been investigated using Raman spectroscopy as a function of temperature from 14 K to 295 K at 1 atm, as well as a function of pressure up to 8.9 GPa at 295 K and up to 6.8 GPa at 120 K. In the range measured, pressure shifts of Raman peaks show no mode softening, indicating a robust and stable material in the Pnma space group. Due to this stability, BaZrS$_3$ serves as an excellent prototype for alloys occupying the same phase but having different unit cell volume. This volume change provides a method for band-gap tuning with the goal of more efficient energy harvesting. Results of these studies will be discussed.