Crystal Structure and Physicochemical Characterization of Novel Lithium-Containing Chalcogenides.

Jennifer Aitken, Ashley Weiland, Christopher Barton and Stanislav Stoyko Duquesne University

Fewer lithium-containing sulfides exist in comparison to other alkali-metal-containing sulfides; yet, lithium-containing sulfides have a number of important potential technological applications including nonlinear optics and lithium-ion batteries. Recent results show impressive second harmonic generation for diamond-like lithium-containing DLSs and initial work demonstrates that these materials may possess significant lithium-ion conductivity and be useful as solid-state electroltyes or electrode materials in solid-state, lithium-ion batteries. In this presentation the structures and physicochemical characterization of several new lithium-containing chalcogenides will be presented. For example, the new compound $\text{Li}_2\text{CdSn}_3\text{S}_8$ adopts a cubic spinel structure where the S^2 - anions create the cubic closest packed array in which the lithium and cadmium/tin cations reside in one eighth of the tetrahedral and half of the octahedral holes, respectively. Another example is the new compound LiMgGeS_3 which adopts a novel noncentrosymmetric structure featuring ethane-like $[\text{Ge}_2\text{S}_6]^4$ - units. Additionally compounds and characterization will be presented.