

EXPLORING THE SYNTHETIC FRONTIERS OF MULTINARY METAL-CHALCOGENIDE SEMICONDUCTORS FOR TUNING THEIR OPTICAL PROPERTIES

P. MAGGARD^a

^a*Department of Chemistry and Biochemistry, Baylor University, Waco, TX, USA*

email address of the presenting author (P. Maggard): Paul_Maggard@baylor.edu

The synthetic preparation of increasingly complex multinary metal-chalcogenides has garnered significant interest with respect to their optical properties, particularly in photovoltaic or second harmonic generation (SHG) applications. Progress in enhancing these properties has arisen from both the manipulation and understanding of the fundamental relationships between their crystalline and electronic structures. Recent synthetic endeavors have discovered new Eu(II)-containing chalcogenides which incorporate coinage metal cations (Cu or Ag) and tetrel cations (Si, Ge, or Sn). These compounds exhibit complex compositions resulting from partial structural disorder and possess noncentrosymmetric structures that currently demonstrate some of the highest mid-IR SHG activities reported. Additionally, results of electronic structure calculations have enabled new insights into the origins of their SHG activity, as well as their small visible-light bandgaps and thermodynamic stability. Furthermore, the presentation will introduce molten-salt synthesis methods for the preparation of other novel Eu(II)-containing chalcogenides, which have begun to illuminate the broader trends and the influence of the main group cations on structural connectivity and electronic structure. Thus, the presentation will focus on the synthetic advancements that have contributed to a deeper understanding of the structure-property relationships in multinary metal chalcogenides.