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Study of bond length as a function of basis set and density functional for As_xS_y glasses[1] LAURA JUDY, JUSTIN OELGOETZ, Austin Peay State University — As_xS_y glasses are used in variety of applications ranging from optical fibers to optoelectronics. Thin films of these materials are known to undergo structural changes when exposed to above-bandgap light as well as γ-radiation. In order to model these effects, one must first establish a validated model which is based on a particular basis set and density functional. This poster presents the results of an ongoing numerical study on the effect of basis set and density functional choice on the bond lengths and angles of AsS clusters, much like what one might find in a As_xS_y glass. Geometry optimization calculations carried out in NWChem using a variety of Pople type (6-311G, 6-311G*, etc.) and Dunning type (cc-pvdz, cc-pvtz, aug-cc-pvdz, aug-cc-pvtz, etc.) basis sets in combination with various density functionals (b3lyp, pbe0, becke88 perdew86, m06, m11, etc.) are being considered. Comparisons of the structural parameters across the calculations as well as comparisons to experimental results will be presented.

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