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First-principles simulations of Raman spectra of As-S glasses CHAMILA DHARMAWARDHANA, KOBLAR JACKSON, Central Michigan University — First principles cluster calculations were used to interpret the experimental Raman spectra of $As_xS_{(1-x)}$ glasses. A large array of cluster models was built to mimic various atomic arrangements and a range of stoichiometries. The dangling bonds on the models were terminated by hydrogen atoms. Using density functional theory, cluster geometries were optimized and vibrational modes and their corresponding Raman/IR activity calculated. $P_xS_{(1-x)}$ models were also studied for comparison. From the cluster energetics, a clear preference for heteropolar bonds was confirmed for both systems. The results of the Raman calculations accounted well for the width of the peaks in the observed spectra and the identities of the main vibrational bands were confirmed. Strong evidence was found for the presence of so called Quasi-Tetrahedral (QT) units as proposed recently by the Boolchand group. The study shows the applicability and predictive capabilities of using cluster calculations in analyzing bulk glasses.

Koblar Jackson
Central Michigan University

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