Ab initio calculation of vibrational frequencies of clusters in \( \text{As}_x\text{S}_{1-x} \) glass and Raman spectra\(^1\) KESHAV SHRIVASTAVA, University of Malaya, V. RADHIKA DEVI, University of Hyderabad, HASAN ABU KASSIM, ITHNIN ABDUL JALIL, University of Malaya, NORHASLIZA YUSOF — We have used the density functional theory (DFT) to calculate the vibrational frequencies from first principles by making clusters of atoms on a high speed computer. We have made the clusters, \( \text{AsS}_4, \text{As}_2\text{S}_3, \text{As}_3\text{S}_2, \text{As}_4\text{S}, \text{AsS}_7, \text{As}_2\text{S}_6, \text{As}_3\text{S}_5, \text{As}_4\text{S}_4, \text{As}_5\text{S}_3, \text{As}_6\text{S}_2, \text{As}_7\text{S}, \text{L-As}_4\text{S}_3, \text{CS-As}_4\text{S}, \text{CS-As}_4\text{S}_4, \text{ES-As}_2\text{S}_6 \) (L=linear zig-zag, CS=corner sharing, ES=edge sharing) and optimized the bond lengths and angles for the minimum energy. The number of computed values of the vibrational frequencies are consistent with \( 3N-3 \), where \( N \) is the number of atoms in a cluster. All of the computed values are tabulated and compared with those found in the Raman spectra of \( \text{As}_x\text{S}_{1-x} \) \((x=0.35-0.45)\) glasses. The experimentally found modes at 183, 221, 355, 371 cm\(^{-1}\) are consistent with those calculated for chain mode-\( \text{As}_4\text{S}_3, \text{As}_3\text{S}_2, \text{As}_2\text{S}_6, \text{AsS}_7 \). In the net work glass the frequencies found are, 195, 206, 227, 351, 369, 371, 388 cm\(^{-1}\) which are consistent with those calculated for, \( \text{As}_7\text{S}, \text{As}_5\text{S}_3, \text{As}_7\text{S}, \text{As}_6\text{S}_2, \text{As}_5\text{S}_3, \text{AsS}_7 \) and \( \text{As}_4\text{S} \). We have previously interpreted the Raman spectra of GeSI galass by this method, V.R. Devi et al, J. Non Cryst. Solids 351,489-494(2005).

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