Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Ab initio calculation of vibrational frequencies of clusters in As $_x$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, AsS_4, As_2S_3, As_3S_2, As_4S, AsS_7, As_2S_6,As_3S_5,As_4S_4,As_5S_3,As_6S_2, As_7S, L-As_4S_3, CS-As_4S,CS-AsS_4,ES-As_2S_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 As_xS_{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-As_4S_3, As_3S_2, As_2S_6, 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, As_7S, As_5S_3, As_7S, As_6S_2, As_5S_3, AsS_7 and As_4S. 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).

[1]Supported by Malaysian Academy of Sciences

Keshav Shrivastava
University of Malaya

Date submitted: 15 Nov 2006 Electronic form version 1.4