Abstract Submitted
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DFT Ab initio Calculation of Vibrational Frequencies in AsSe glass KESHAV SHRIVASTAVA, HASAN KASSIM, AHMAD NAZRUL ROSLI, University of Malaya, JABATAN FIZIK COLLABORATION — By using DFT double zeta wave functions, we calculated the structure, bond length (picometer, pm), frequencies(intensities)[degeneracy] for various clusters of arsenic selenide. Our results are as follows. (i) AsSe(diatomic) bond length 216pm, 244.0(1/cm). (ii) As_2Se(linear) bond length 228.5 pm, frequencies 27.6(1.9) and 387.6(4.3). (iii) As_2Se(triangular) As-Se 243.4 pm, As-As 223.3 pm, frequencies 237.3(2.4) and 332.4(0.05)(1/cm). (iv) As_3Se (triangular) bond length 238.4 pm, frequencies 107.5 and 296(weak)(1/cm). (v) As_4Se (square) bond length 250.2 pm, 58.5(0.04), 241.3(5.9)(1/cm). (vi) $AsSe_3$ (triangular), bond length 231.2 pm, 75.9(0.003), 103.5(1.26)[2], 350.9(33.2)[2]. From this study we identify that linear As-Se-As for which the calculated frequency is 27.6(1/cm) is in agreement with the data of Nemanich, Phys. Rev. B 16, 1655(1977), J. C. Phillips et al Phys. Rev B 21, 5724(1980). We have successfully calculated several vibrational frequencies accurately which agree with the Raman data.

1. V. R. Devi et al J. Non-Cryst. Solids 351, 489(2005);353,111(2007)

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