Abstract Submitted
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Electronic Structure and Vibrational spectra of C_2B_{10} Based Clusters and Films[1] L. L. BOYER, KYUNGWHA PARK, M. R. PEDERSON, Naval Research Laboratory, W. N. MEI, X. C. ZENG, S. BULUSU, ELLEN DAY, SHIREEN ADENWALLA, University of Nebraska, SEAMUS CURRAN, JAMES DEWALD, New Mexico State University — Semiconducting boron carbide films can be used to detect neutrons and convert energy of associated nuclear reactions directly into electrical current. Such films were prepared by removing hydrogen from the three polytypes of $C_2B_{10}H_{12}$ (carborane) deposited on various surfaces. Results from Raman scattering measurements on these films will be presented and compared with results of calculations for clusters. The electronic structure, total energy and vibrational properties of carborane molecules and C_2B_{10} clusters calculated using density functional theory are reported. Computed vibrational spectra for carborane molecules are found to be in close agreement with previously published measured spectra taken on carborane solids. Eleven vibrationally stable C_2B_{10} clusters have been identified and their relative energies, HOMO-LUMO gaps and vibrational properties will be discussed. Good agreement with the experimental Raman spectra is achieved from theoretical spectra computed using a Boltzmann distribution of the six lowest energy free-clusters.

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