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Calculated Properties of $B_{10}C_2$ Clusters[1] L. L. BOYER, KYUNG-WHA PARK, M. R. PEDERSON, Naval Research Laboratory, Washington DC 20375, W. N. MEI, R. F. SABIRIANOV, Department of Physics, University of Nebraska, Omaha, NE 68182, XIAO CHENG ZENG, Department of Chemistry, University of Nebraska, Linclon, NE 68588, LUIS G. ROSA, S. BALAZ, P. A. DOWBEN, Department of Physics, University of Nebraska, Lincoln, NE 68588 —
The electronic structure, total energy and vibrational properties of clusters formed by removing hydrogen from $B_{10}C_2H_{12}$ are studied using density functional methods and semi-empirical models. Properties of several metastable structures, formed using density functional methods, are compared with analogous results from model calculations and available experimental data, including photoemission, optical properties, and infra-red spectroscopy. We consider our work to be a first step toward understanding the interesting properties of semiconducting films formed by removing hydrogen from films of meta- ortho- and para- carborane, the three polytypes of $B_{10}C_2H_{12}$, deposited on metal surfaces. Agreement between experiment and theory for the carborane source molecules has been established.

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