

Abstract Submitted
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Computational Studies of Nanostructures of Boron P. TANDY, M.

YU, C. LEAHY, University of Louisville, W.Q. TIAN, Jilin University, S.Y. WU, C.S. JAYANTHI, University of Louisville, U. OF LOUISVILLE/JILIN U. TEAM — The goal of this work is to develop a reliable semi-empirical Hamiltonian for boron that may be used to predict nanostructures of boron. It is well known that bonding in boron is complicated as it may form three-center, two-electron bonds. The semi-empirical Hamiltonian used here was recently developed by Leahy *et al.* in the framework of linear combination of atomic orbitals[1]. The salient feature of this Hamiltonian is that it treats environment dependency and charge redistributions on equal footing. It will be shown that such a parameterized Hamiltonian can predict the B₈₀ cage structure with C₁ symmetry as found in a recent first-principles study [2]. Having validated our semi-empirical Hamiltonian for boron with small boron clusters and the B₈₀ cage, we have performed a systematic study of other boron nanostructures: (i) larger cage structures (*e.g.*, B₂₁₅), (ii) boron clusters cut from the bulk alpha boron, and (iii) boron sheets (triangular sheets with and without holes). We will discuss the ground state structures of these boron nanostructures as well as the energetics and HOMO-LUMO gaps of different families of boron clusters as a function their diameters. 1. C. Leahy *et al.* Phys. Rev. B74, 155408 (2006). 2. N. G. Szewacki *et al.* PRL 100, 159901 (2008).

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