Abstract Submitted
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Simulations of the Structure and Properties of Large Icosahedral Boron Clusters Based on a Novel Semi-Empirical Hamiltonian[1] PAUL TANDY, MING YU, C.S. JAYANTHI, SHI-YU WU, University of Louisville, CONDENSED MATTER THEORY GROUP TEAM — A successful development of a parameterized semi-empirical Hamiltonian (SCED-LCAO) for boron based on a LCAO framework using a sp^3 basis set will be discussed. The semi-empirical Hamiltonian contains environment-dependency and electron screening effects of a many-body Hamiltonian and allows for charge self-consistency. We have optimized the parameters of the SCED-LCAO Hamiltonian for boron by fitting the properties (e.g., the binding energy, bond length, etc.) of boron sheets, small clusters and boron alpha to first-principles calculations based on DFT calculations. Although extended phases of boron alpha and beta have been studied, large clusters of boron with icosahedral structures such as those cut from boron alpha are difficult if not impossible to simulate with ab initio methods. We will demonstrate the effectiveness of the SCED-LCAO Hamiltonian in studying icosahedral boron clusters containing up to 800 atoms and will report on some novel boron clusters and computational speed. [1] C. Leahy, et al, Phys. Rev. B 74,155408 (2006). [2] P. Tandy, et al, Bulletin of the APS, 2009 APS March Meeting Vol. 54, Num.1, Sess. D26, [3] Ming Yu, et al, J. Chem. Phys. 130,184708 (2009). [4] Ming Yu, S.Y. Wu, and C.S. Jayanthi, Physica E 42, 1 (2009).

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