Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Development of a Semi-empirical Hamiltonian for Boron and the Prediction of Structures for Intermediate-Size Boron Clusters PAUL TANDY, CHRIS LEAHY, University of Louisville, JAMES SIMRALL, YU MING, University of Louisville, CHAKRAM JAYANTHI, SHI-YU WU, University of Louisville — In this work, we will present a semi-empirical Hamiltonian for Boron that includes environment-dependent terms and electron correlation terms with the on-site charge calculated self-consistently. This Hamiltonian developed within the LCAO framework has been shown previously to be successful in predicting the properties of intermediate-size silicon and carbon clusters, silicon nanowires and carbon nanotubes, and surface reconstructions of Si(100) and Si(111) surfaces [1]. One of the goals of this work is to obtain the parameterized Hamiltonian for Boron by fitting the properties of small boron clusters ($B_2$to B_6) and of the bulk phases of Boron, as obtained by our method, to ab-initio calculations [2,3]. The optimized parameters for Boron will be used to predict the structure and stability of intermediate-size Boron clusters. [1] C. Leahy, M. Yu, C.S. Jayanthi, and S.Y. Wu, Phys. Rev. B 74, 155408 (2006) [2] G. Kresse and J. Furthmuller, Phys. Rev. B 54, 11169 (1996). [3] M. J. Freese et al., Gaussian 03, Gaussian Inc. (2004).

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Date submitted: 04 Dec 2007 Electronic form version 1.4