

Abstract Submitted
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Bonding in elemental boron: a view from electronic structure calculations using maximally localized Wannier functions TADASHI OGITSU, Lawrence Livermore National Laboratory, FRANCOIS GYGI, University of California, Davis, JOHN REED, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, GIULIA GALLI, University of California, Davis — Boron exhibits the most complex structure of all elemental solids, with more than 300 atoms per unit cell arranged in interconnecting icosahedra, and some crystallographic positions occupied with a probability of less than one. The precise determination of the ground state geometry of boron—the so-called β -boron structure—has been elusive and its electronic and bonding properties have been difficult to rationalize. Using lattice model Monte Carlo optimization techniques and *ab-initio* simulations, we have shown that a defective, quasi-ordered β solid is the most stable structure *at zero* as well as finite T. In the absence of partially occupied sites (POS), the perfect β -boron crystal is unstable; the presence of POS lower its internal energy below that of an ordered α -phase, *not mere an entropic effect*. We present a picture of the intricate and unique bonding in boron based on maximally localized Wannier (MLWF) functions, which indicates that the presence of POS provides a subtle, yet essential spatial balance between electron deficient and fully saturated bonds. This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/ LLNL under contract no. W-7405-Eng-48.

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