Abstract Submitted
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The Structure, Stability, and Properties of a One-Dimensional α-Boron Structure[1] CHERNO BABA KAH, PAUL TANDY, MING YU, C.S. JAYANTHI, S.Y. WU, University of Louisville, CONDENSED MATTER THEORY GROUP TEAM — Boron is an electron deficient element exhibiting a complex and versatile chemistry. In this work we have performed a preliminary study on the structural stability and electronic properties of one-dimensional α-boron structures based on the SCED-LCAO molecular dynamics scheme (MD) [PRB 74, 15540 (2006)]. The one-dimensional α-boron structures were generated by constructing icosahedra B_{12} clusters, referred as α-boron balls, and arranging them in one-dimension. Such structures were stabilized through the simulated annealing based on the SCED-LCAO MD. We found that: (1) the α-boron ball is compressed in comparison to its bulk counterpart (α-phase); (2) the distance between "α-boron balls" is shorter in the center of the chain than that at the two ends and decreases as the length of the chain increases; (3) the HOMO-LUMO gap is very small ($\sim$1 meV) in the finite chains, but it opens up when the chain length becomes infinite. The optimized lattice constant of the infinite α-boron chain was found to be 2.998 Å and its energy gap is found to be 0.74 e. The stability and properties of ring-shaped one-dimensional α-boron structures will also be discussed.

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