Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

A molecular dynamics study on the structural and electronic properties of two-dimensional icosahedral B12 cluster based structures[1]
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— Our previous study on one-dimensional icosahedral B12 cluster (α-B12) based chain [Bulletin of APS Annual Meeting, p265 (2013)] and ring structures has prompted us to study the two-dimensional (2D) α-B12 based structures. Recently, we have carried out a systematic molecular dynamics study on the structural stabilities and electronic properties of the 2D α-B12 based structures using the SCED-LCAO method [PRB 74, 15540 (2006)]. We have considered several types of symmetry for these 2D structures such as δ3, δ4, δ6 (flat triangular), and α' types. We have found that the optimized structures are energetically in the order of δ6 $<\alpha$' $<\delta$3 $<\delta$4 which is different from the energy order of α'$<\delta$6 $<\delta$4 $<\delta$3 found in the 2D boron monolayer sheets [ACS Nano 6, 7443 (2012)]. A detailed discussion of this study will be presented.

[1]The first author acknowledges the McSweeny Fellowship for supporting his research in this work.

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Date submitted: 11 Nov 2013 Electronic form version 1.4