

Abstract Submitted
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Growth of Monolayer Boron Sheet on Metal and Metal Boride Surface YUANYUE LIU, QINGBO YAN, Dept. of Mech. Eng. & Mat. Sci., Rice U., HOONKYUNG LEE, Dept. of Mech. Eng. Mat. Sci., Rice U., BORIS YAKOBSON, Dept. of Mech. Eng. & Mat. Sci., Rice U., COMPUTATIONAL MATERIALS SCIENCE TEAM — Monolayer boron (B) sheet has attracted lots of interests recently due to its metallic conductivity. However, their experimental synthesis has not been achieved so far, which calls for theoretical investigation. Using first principles calculations, we study the possibility of growing monolayer B sheets on metal (Ag, Au) and metal boride (MgB₂, TiB₂) surface as catalytic substrate. It is shown that after decomposition from precursor, B atoms will aggregate to cluster, then to sheets, while three dimensional bulky B is prohibited due to high nucleation barrier. Charge transfer between substrate and B sheet shifts its stability dependence on hexagon vacancy density. B sheet with specific vacancy density can have cleavage energy as small as graphite thus should be easily peeled off. This work suggests promising approach to synthesize B sheets and would possibly pave the way towards their applications to electronic, optic, and mechanic nano-devices.

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