

**Insertion of Line Defect in Nanoribbons of Graphene, Boron Nitride, and Hybrid of Them:
An AIMD Study**

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Using constant-temperature ab initio molecular dynamics simulation we demonstrated a way to insert extended line defects (ELDs) at the grain boundary in hybrid graphene and boron nitride nanoribbons (BNCNRs) as well as in pure graphene nanoribbons (GNRs) and pure boron nitride nanoribbons (BNNRs). Our systematic studies have shown that 5-8-5 and 8-8-8 extended line defects can be installed and stabilized by depositing different adatoms such as carbon, boron, and nitrogen at the grain boundaries of graphene–graphene, boron nitride–boron nitride, and graphene–boron nitride junctions. The electronic and magnetic structures of these nanoribbons are highly modulated in the presence of these ELDs.

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