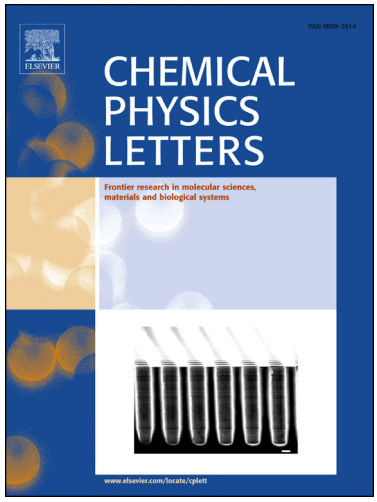

Research paper

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Towards a metal-semiconductor transition in two dimensions

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Abstract

Two-dimensional (2D) heterosheets built from silicon and boron may exhibit an intrinsic metallic behavior. From density-functional-theory computer simulations, we have demonstrated that a 2D honeycomb binary compound (h-SiB), which exhibits robust structural and thermal stabilities, maintains its metallicity by increasing hydrogen coverages of 25%, 50%, and 75% on boron or silicon sublattices. However, under a total hydrogenation condition (100%) on B or Si sites, h-SiB opens a well-defined bandgap, meaning that it is possible to obtain a metal-insulator transition at zero temperature in 2D. Additional calculations show that the hydrogenation on B sublattices is energetically more favorable than on silicon.

Keywords: 2D SiB sheets; metallic behavior; hydrogenation; metal-insulator transition

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