

Abstract Submitted
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Electronic structure of partially hydrogenated graphene superlattices JOO-HYOUNG LEE, JEFFREY GROSSMAN, Massachusetts Institute of Technology — First-principles calculations based on density functional theory are performed to investigate the electronic structure of graphene-graphane superlattices (GSLs) by varying the widths of both the graphene and graphane regions. For the armchair-type interface between the graphene and graphane strips (AGSLs), the superlattices become semiconducting with a band gap exhibiting a similar dependence on the width of the graphene region as in armchair graphene nanoribbons. In contrast with the nanoribbons, however, the band gap of AGSLs shows both direct and indirect characteristics, depending on the graphane width. On the other hand, GSLs with a zigzag interface (ZGSLs) possess magnetic ground states except for those with a very narrow graphene strip. While an anti-ferromagnetic (AFM) phase is found to be energetically more stable than the ferromagnetic (FM) one, the energy difference between the two phases is so small (< 10 meV) that these two phases become nearly degenerate. These findings point toward an alternative route for graphene-based applications without requiring physical cutting as in graphene nanoribbons.

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