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Orientationally Misaligned Zipping of Lateral Graphene and Boron Nitride Nanoribbons with Minimized Strain Energy and Enhanced Half-Metallicity[1] JIANG ZENG, Univ of Sci Tech of China, WEI CHEN, Harvard University, PING CUI, Univ of Sci Tech of China, DONG-BO ZHANG, Beijing Computational Science Research Center, ZHENYU ZHANG, Univ of Sci Tech of China — Lateral heterostructures of two-dimensional materials may exhibit various intriguing emergent properties. Yet when specified to the orientationally aligned heterojunctions of zigzag graphene and hexagonal boron nitride (hBN) nanoribbons, realizations of the high expectations on their properties encounter two standing hurtles. First, the rapid accumulation of strain energy prevents largescale fabrication. Secondly, the pronounced half-metallicity predicted for freestanding graphene nanoribbons is severely suppressed. By properly tailoring orientational misalignment between zigzag graphene and chiral hBN nanoribbons, here we present a facile approach to overcome both obstacles. Our first-principles calculations show that the strain energy accumulation in such heterojunctions is significantly diminished for a range of misalignments. More strikingly, the half-metallicity is substantially enhanced from the orientationally aligned case, back to be comparable in magnitude with the freestanding case. The restored half-metallicity is largely attributed to the recovered superexchange interaction between the opposite heterojunction interfaces. The present findings may have important implications in eventual realization of graphene-based spintronics.

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