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Strain Engineering of Graphene: Atomistic Simulation of Y-junctions and Nanobubbles[1] ZENAN QI, Boston University, DARIO BAHAMON, National University of Singapore, HAROLD PARK, Boston University, VITOR PEREIRA, National University of Singapore, DAVID CAMPBELL, Boston University, ANTONIO CASTRO NETO, National University of Singapore and Boston University — We have studied the effects of two and three-dimensional states of strain on electronic transport in monolayer graphene. Using a combined atomistic simulation approach with molecular mechanics, molecular dynamics, tight binding exact diagonalization and Landauer-Büttiker formulism, we have explored how various deformation patterns induce tunable pseudomagnetic field (PMF) distributions and furthermore how the Landau levels arising from PMF affect the quantum transport properties. Specifically, graphene Y-junction structures are found, under triaxial strains, to behave like pseudomagnetic quantum dots that selectively guide electron movement; valley degeneracy is broken when both strain-induced PMF and external real magnetic fields are present. Furthermore, graphene nano-bubbles with different geometries obtained by gas pressure can also be controlled as functional blocks due to PMF-restricted quantum transport by manipulation of strain. The simulation results show the promising potential to utilize graphene as a tunable building block for electronic NEMS/MEMS devices by strain engineering.

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Zenan Qi
Boston University

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