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First-Principles Calculations of Graphene Nanomesh WILLIAM OSWALD, ZHIGANG WU, Colorado School of Mines — Graphene has recently attracted intensive attentions owing to its remarkable structural and electronic properties and its significant potential for applications in electronic and optoelectronic devices for size miniaturization and fast electron transportation. However, bulk graphene is a semi-metal with zero bandgap E_g, and opening a sizable E_g is critical for building operational graphene-based transistors. Recently, a new scheme of opening bandgap through punching nanoscale holes in graphene sheet, the graphene nanomesh, was proposed and verified experimentally [1]. However, the mechanism leading to the bandgap opening remains unknown. We have carried out first-principles calculations based on density functional theory (DFT) to study the bandgap opening mechanism and E_g as functions of structural parameters, including the hole size, the hole shape, and the hole-hole distances. Our results suggest that the bandgap opening is a result of quantum confinement at nanomesh necks, while the value of E_g depends not only on the width of nanomesh necks, but also on the chirality of the hole edge. This work was supported by the start-up research funds from Colorado School of Mines.

[1] J. Bai, X. Zhong, S. Jiang, Y. Huang, and X. Duan, Nature Nanotech. **5**, 190 (2010).

Zhigang Wu
Colorado School of Mines

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