Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Band-gap switching and scaling of nanoperforated graphene. HAIYUAN CHEN, XIAOBIN NIU, University of Electronic Science and Technology of China, Chengdu 610054, PR China, INTERNATIONAL CENTER FOR ARTIFICIAL MATERIALS TEAM — A framework of {w1, w2, R}classification for constructing the graphene nanomesh (GNM) of zigzag-edged hexagonal nanohole is systematically built. Three integer indexes w1, w2, and R indicate the distances between two neighboring sides of nanoholes in two directions and the nanohole size respectively, which leading to a straightforward gap opening criteria, i.e., w_1+w_2-R=3n+1,n∈Z, steered via DFT band structure calculations. The guiding rule indicates that the semimetallic and semiconducting variation is consistent with a peculiar sequence 010 and 100 (0/1 represent gap closure/opening) with a period of 3 for odd and even w1 respectively. The periodic nanoperforation induced gap sizes agree with a linear fitting with a smaller $\sqrt{}$(N_rem)/N_tot ratio, while deviates from that when (w_1+w_2)<R+1. Particularly, the {p, 1, p}and {1, q, q}structures demonstrate each unique scaling rule pertaining to the nanohole size only when n is set to zero. Furthermore, the coexistence of Dirac and flat bands is observed for {1, q, q}and {1, 1, m}structures, which is sensitive to the atomic patters.

Haiyuan Chen
University of Electronic Science and Technology of China, Chengdu 610054, PR China

Date submitted: 09 Nov 2016 Electronic form version 1.4