Band-gap switching and scaling of nanoporous 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 \( \{w_1, w_2, R\} \) classification for constructing the graphene nanomesh (GNM) of zigzag-edged hexagonal nanohole is systematically built. Three integer indexes \( w_1, w_2, \) 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., \( w_1+w_2-R=3n+1, n \in \mathbb{Z} \), 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 \( w_1 \) respectively. The periodic nanoporation induced gap sizes agree with a linear fitting with a smaller \( \sqrt{N_{\text{rem}}}/N_{\text{tot}} \) 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 pattern.