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First principles study of edge effects in electronic structures of graphene nanoflakes and nanoribbons CHENGBO HAN, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, Raleigh, NC, CENTER FOR HIGH PERFORMANCE SIMULATION (CHIPS) TEAM — Graphene is a promising material for future nanoelectronics. Understanding of the edge effects on the electronic structure of graphene nanoflakes and nanoribbons is important for its nanoscale applications. Using the real space multigrid method within density functional theory, we systematically simulate STM images of nanoflakes and nanoribbons with both zigzag and armchair edges. Our results explain several STM patterns seen in experiments [1], such as triangular and hexagonal lattices for different shapes of flakes. We also find that localization of edge states in zigzag flakes depends on the interior angle between two edges. Furthermore, we show that the influence of Si(001)-2x1-H substrate on the local density of states of graphene nanoflakes is not significant when the graphene layer is 0.3 nm above the substrate.

[1] K. A. Ritter and J. W. Lyding, Nature Materials 8, 235 (2009).

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