Abstract Submitted for the MAR16 Meeting of The American Physical Society

Decay patterns of edge states at reconstructed armchair graphene edges¹ CHANGWON PARK, ORNL, USA, JISOON IHM, Seoul National Univ., Korea, GUNN KIM, Sejong Univ., Korea — Density functional theory calculations are used to investigate the electronic structures of localized states at reconstructed armchair graphene edges. We consider graphene nanoribbons with two different edge types and obtain the energy band structures and charge densities of the edge states. By examining the imaginary part of the wave vector in the forbidden energy region, we reveal the decay behavior of the wave functions in graphene. The complex band structures of graphene in the armchair and zigzag directions are presented in the first-principles framework.

¹G.K. acknowledges the support of the Basic Science Research Program through the National Research Foundation of Korea funded by the Ministry of Education (Grant No. 2013R1A1A2009131) and the Priority Research Center Program (Grant No. 2010-0020207).

Gunn Kim Sejong Univ., Korea

Date submitted: 06 Nov 2015 Electronic form version 1.4