Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Stability and Electronic Structures of Al-, Si- and Au-incorporated Divacancy Graphenes: A First-principles Study NA-YOUNG KIM, EUI-SUP LEE, YONG-HYUN KIM, Graduate School of Nanoscience and Technology (WCU), KAIST, Daejeon 305-701 — C, N, and O decorated divacancy pores in graphene have been reported as well. Especially, the N4 divacancy pore can strongly bind with the divalent 3d transition metals (TMs) because of the large enough pore size and the strong p-d hybridization. Recently, the Si- and Au-incorporated divacancy pore have been also proposed, but understanding of the stability or electronic properties is largerly lacking. In this work, we invesgated the stability and electronic structure of Al-, Si- and Au-incoporated divacancy graphenes decorated with reactangular CmNn, NnOl, and OlCm, based on first-principles density-functional theory (DFT) calculations. We found that the Al-CN3, Si-C2N2, and Au-CN3 are most stable configurations for each cations because the unpaired electrons of edge atoms of divacancy pore could be completely passivated. The binding energies are also higher than cohessive energies due to the strong p-p or p-d hybridization. Because of the strong hybridizaition, the restoration of π-network of graphene or small band-gap opening near the fermi-level are also observed.

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Date submitted: 27 Nov 2012 Electronic form version 1.4