Hisaki Sawahata

Mina Maruyama and Susumu Okada

Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba 305-8571, Japan

hsawahata@comas.frsc.tsukuba.ac.jp

Energetics and electronic properties of B_3N_3-doped graphene: Semiconducting graphene heterostructures

Electronic structures of porous sp^2 carbon networks strongly depend on their network topology and an arrangement of the pores, making them a semiconductor or metal. In addition to pores, interfaces with other two-dimensional materials also modulate the electronic structure of graphene depending on the interface shape and constituents. These facts open a question whether the energetics and electronic structure of porous graphene are further tunable by filling pores with nanoflakes of other two-dimensional materials. Among various two-dimensional materials, h-BN is an appropriate dopant. Thus, in this work, we aim to investigate the energetics and electronic structure of B_3N_3-doped graphene in which B_3N_3 (borazine) is embedded into the graphene nanomeshes consisting of triangularly arranged hexagonal vacancies, using the density functional theory with the generalized gradient approximation.

Figure 1 shows an optimized structure of the representative B_3N_3-doped graphene. The doped B_3N_3 rings form triangular lattice in graphene network by forming the heterobonds of BC and NC at their borders. Figure 2 shows the total energy of B_3N_3-doped graphene as a function of the spacing between adjacent B_3N_3 domains. The total energy is found to be inversely proportional to B_3N_3 spacing. Furthermore, the energy also weakly depends on the network topology of the graphene domain. The heterosheets with the Kekulé structure have lower total energy than the other heterosheets for the same B_3N_3 spacing. The network topology of the graphene region also affects the electronic structures of B_3N_3-doped graphene. Figure 3 shows the band gap of the heterosheets as a function of the spacing between adjacent B_3N_3 domains, indicating that all sheets are semiconductors with finite energy gap irrespective of the arrangements of B_3N_3 in graphene. The gap monotonically decreases with increasing the B_3N_3 spacing. The heterosheets with the Kekulé structure have a direct gap at the Γ point, while the remaining heterosheets have direct gap at K point. Calculated band gap for the heterosheet with the Kekulé structure is narrower than that with the non-Kekulé structure for the same B_3N_3 spacing.
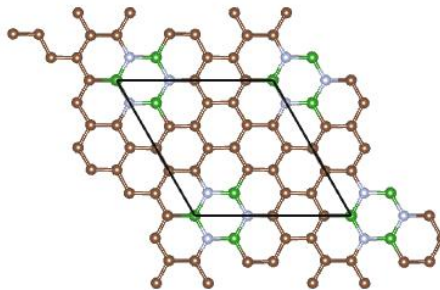

Figure 1: Optimized structure of B_3N_3-doped graphene. Brown, green, and cyan circles denote C, B, and N atoms, respectively.

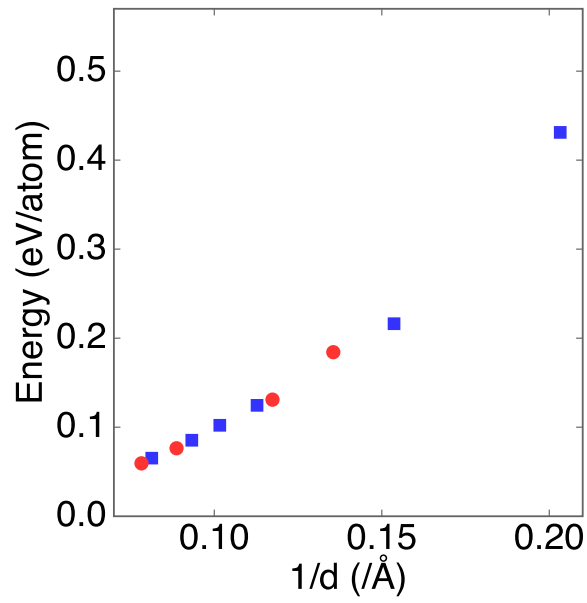**Figure 2:** Total energy of B$_3$N$_3$-doped graphene as a function of the inverse of the B$_3$N$_3$ spacing. Circles and squares denote the energy of the heterosheets with and without the Kekule structures, respectively.
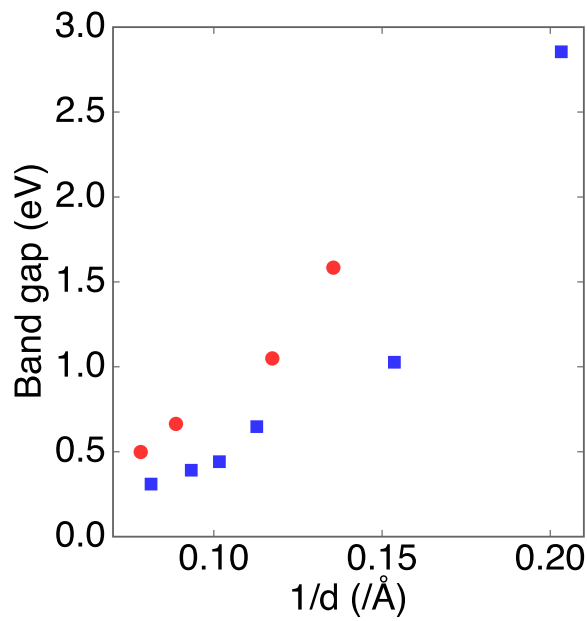

Figure 3: Band gap of B$_3$N$_3$-doped graphene as a function of the inverse of the B$_3$N$_3$ spacing. Circles and squares denote the energy of the heterosheets with and without the Kekule structures, respectively.