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Achieving robust n-type nitrogen-doped graphene via a binary-doping approach HYO SEOK KIM, HAN SEUL KIM, SEONG SIK KIM, YONG-HOON KIM[1], Korea Advanced Institute of Science and Technology — Among various dopant candidates, nitrogen (N) atoms are considered as the most effective dopants to improve the diverse properties of graphene. Unfortunately, recent experimental and theoretical studies have revealed that different N-doped graphene (NGR) conformations can result in both p- and n-type characters depending on the bonding nature of N atoms (substitutional, pyridinic, pyrrolic, and nitrilic). To overcome this obstacle in achieving reliable graphene doping, we have carried out density functional theory calculations and explored the feasibility of converting p-type NGRs into n-type by introducing additional dopant candidates atoms (B, C, O, F, Al, Si, P, S, and Cl). Evaluating the relative formation energies of various binary-doped NGRs and the change in their electronic structure, we conclude that B and P atoms are promising candidates to achieve robust n-type NGRs. The origin of such p- to n-type change is analyzed based on the crystal orbital Hamiltonian population analysis. Implications of our findings in the context of electronic and energy device applications will be also discussed. This work was supported by the Basic Science Research Grant (No. 2012R1A1A2044793), Global Frontier Program (No. 2013-073298), and Nano-Material Technology Development Program (2012M3A7B4049888) of the National Research Foundation funded by the Ministry of Education, Science and Technology of Korea.

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