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The electronic structure and chemical bonding of graphene doped with Group IA and Group VIIA elements: A density functional theory study YIMING MI, Graduate Department, Shanghai University of Engineering Science, SHUICHI IWATA, Graduate School of Frontier Sciences, The University of Tokyo — The ground state geometry and the electronic structure of graphene doped with group IA and VIIA elements were calculated with the first principles plane wave pseudopotential approaches within the density functional theory formalism in this paper. In terms of the generalized gradient approximation(GGA), GW approximation and optimizing atomic positions, a reliable geometry of the structure was acquired. The calculated formation energies for different configurations under ambient temperature implied that a new kind of material will produce. The results acquired here allow one to suggest new material with semiconductor or semimetallic behavior by adjusting the relative concentration of the doped atoms carefully.

Yiming Mi
Graduate Department, Shanghai University of Engineering Science

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