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High free carrier density in aluminum adsorbed graphene YU-TSUNG LIN, MING-FA LIN, Department of Physics, National Cheng Kung University — Electronic properties of graphene are enriched by aluminum adsorption on surface. The Al adsorbate could be used in n-type transfer doping in graphene. From the first-principle density functional calculations, performed by Vienna ab initio simulation package, there are lots of free conduction electrons in the distorted Dirac-cone structure. Charges transferred from Al to C atoms are about 1.24 e, almost irrespective of the concentration and distribution of the adatoms. A high carrier density is estimated to be $\sim 6\times 10^{-14}/\mathrm{cm}^2$ for a ratio of Al/C = 12.5%. Such carriers mainly originate from the hybridization of Al $3s$ and C $2p_z$ orbitals, as clearly indicated from the orbital-projected density states, charge distributions and atom-dominated energy bands. Aluminum adsorbed graphene is predicted to have the highest free carriers density except for Al/C $\geq 25\%$ compared with the other adatom-adsorbed systems.

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