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First-principles investigation of lithium doped of bilayer graphene and Lithium Intercalated Carbon Nanotubes OGUZ GULSEREN, HUSEYIN SENER SEN, Bilkent University — We have performed first-principles calculations based on density-functional theory for understanding of the structural and electronic properties of Li doped bilayer graphene and Li intercalated CNTs especially addressing the controversial charge transfer state between Li and C. We have checked the possible adsorption, substitution and intercalation of Li by using a bilayer graphene system both with AB stacking (12 different initial configurations) and AA stacking (8 different initial configurations). All calculations are repeated both with LDA and GGA exchange-correlation potential, even though the values of binding energies are different, their order and corresponding physical picture are same from both of the functionals as well as the stackings. In conclusion, we can summarize that Li prefers the hollow site adsorption geometry and it prefers intercalation but not the substitution. In these adsorption modes, almost 0.9 electron of Li atom is transferred to neighboring carbon atoms network leaving positively charged core behind.

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