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First-principle study on substrate-induced structures of bismuth adsorption on graphene. SHIH-YANG LIN, Department of Physics, National Cheng Kung University, SHEN-LIN CHANG, Department of Electrophysics, National Chiao Tung University, HSIN-HSIEN CHEN, SHU-HSUAN SU, JUNG-CHUN HUANG, MING-FA LIN, Department of Physics, National Cheng Kung University — The geometric and electronic properties of Bi-adsorbed monolayer graphene, enriched by the strong effect of substrate, are investigated by the first-principles calculations. The six-layered substrate, corrugated buffer layer, and slightly deformed monolayer graphene are all simulated. Adatom arrangements are optimized through detailed analyses on adsorption energies and ground-state energies of various adsorption sites, revealing a hexagonal array of Bi atoms dominated by the interactions between buffer layer and monolayer graphene. The increasing temperature can overcome a ˜50 meV energy barrier and induce triangular and rectangular nanoclusters. The most stable and the metastable structures agree with the scanning tunneling microscopy measurements. The density of states exhibits a finite value at the Fermi level, a dip at low energy, and a shoulder at ˜-0.8 eV, as observed in the experimental measurements of tunneling conductance.

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