NT-P13

Binding strength and Wetting Properties of Metal Nanoparticles on Carbon Nanotubes and Graphene

Noejung Park[1], Seokho Lim[1], Seungho Moon[2]

[1]Department of Applied Physics, Dankook University
[2]Samsung Corning Co., Suwon 443-732, South Korea

Adsorption geometries and binding strength of metal nanopoarticles (Al, Au, Pd, Pt, Ti) on carbon nanotubes and graphene are investigated through the density-functional theory (DFT) calculation. Adsorption energetics depends not only on the type of element but also on the size of particles. The accumulated aluminum and gold nanoparticles are likely to form a (111)-like metal surface, where the metal-carbon bond becomes energetically unstable. Meanwhile, the palladium, platinum, and titamium particles strongly chemisorb on the nanotube surface inducing serve reconstructions. We show that the boron or nitrogen doping in the graphite layer substantially increase the al binding strength