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Structure and electronic properties of alkali and alkaline-earth metals on graphene[1] JIAN ZHOU, Virginia Commonwealth University, SHUNHONG ZHANG, QIAN WANG, QIANG SUN, Peking University, PURUSOTTAM JENA, Virginia Commonwealth University — A thorough search of the monolayer structure of Li, Na, K, and Ca atoms on graphene, based on a synergistic combination of density functional theory and particle swarm optimization algorithm, yielded unusual deposition patterns. For Li atoms, we show that they prefer to cluster on graphene, irrespective of their concentration. We further show that an external electric field applied vertically to the graphene surface or doping with boron can prevent this clustering, leading to the homogeneous growth of Li. For larger atoms Na, K, and Ca, they distribute uniformly when their coverage ratio M:C is 1:6, but the Na and Ca atoms self-assemble to form parallel quasi-one-dimensional chains when their coverage is reduced to 1:8. Electron-phonon coupling calculations further show that the NaC_6 is a superconductor with critical temperature of 5.8 K. At low concentration (M:C = 1:8) and depending on metal species, well-aligned atomic metal chains interact with graphene with varying intensity, making it possible to achieve either rigid or non-rigid band doping in graphene.

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