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Ab initio study of alkali metals adsorption with varying coverage on graphene KYUNG-HWAN JIN, SEON-MYEONG CHOI, SEUNG-HOON JHI, Department of Physics, POSTECH, Republic of Korea — Graphene exhibits many interesting physics and promises potential application to electronic devices. In addition, graphene is considered as a supporting template for catalysts and hydrogen storage. Understanding the contact of graphene with metal is one of key processes in such applications. We carried out first principles calculations to study electrical properties of graphene with adsorption of alkali metals at varying coverage. The adsorption energy and distance, the charge transfer and the Fermi level shift of graphene are particularly investigated as the coverage of metals is changed. It is found that the charge transfer from the metal to graphene shows a strong coverage dependence, which is fit into a model that incorporate the graphene electronic structure and the Coulomb interaction of metal-graphene and metal-metal.

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