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First-Principles Study of Contact Resistance between Graphene and Metal Electrodes[1] TOMOAKI KANEKO, Computational Materials Science Unit, NIMS, TAKAHISA OHNO, Computational Materials Science Unit, NIMS, Institute of Industrial Science, University of Tokyo — Graphene attracts much interest for post-silicon electronics material due to its outstanding electronic transport properties such as considerably high mobility at room temperature. For the application of electronics devices, contacting of metal electrodes is necessary and decreasing of contact resistance between graphene and the metal electrodes is regarded as one of a key issue. In this study, we investigate the contact resistance using DFT+NEGF method. We consider the Ni and Cu electrode within LDA and TM-type norm-conserving pseudo-potential. We employed PHASE code [1] to determine the interface structures. Then, we constructed two terminal device structures in which current flows from metals to graphene. The electron transport properties were calculated using ASCOT code[2]. For Ni electrode, the dependence of the electrode size qualitatively agrees well with that obtained by the experiments. But our results suggest that contact resistance can be reduced considerably. [1] http://www.ciss.iis.u-tokyo.ac.jp/english/project/device/. [2] H. Kondo, J. Nara, H. Kino and T. Ohno, Jpn. J. Appl. Phys. 47, 4792 (2008).

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