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Metal selection criteria for enhancing electrical conductance of metal-graphene junctions MARCELO KURODA, Univ. of Illinois - IBM T.J. Watson, J. TERSOFF, IBM T.J. Watson R.C., DENNIS NEWNS, IBM T.J. Watson, GLENN MARTYNA, IBM T.J. Watson R.C. — We study from first principles the electrical conductance of a junction formed by graphitic films in between metal electrodes. We find that for some metals the junction conductance decays exponentially with the number of graphene layers (thickness of the film) while for others it saturates. These different behaviors are attributed to the presence/absence of Fermi-level states in the metal electrode that couple to those of the graphitic thin film. We also find that the bonding between the metal and graphene atoms at the interface has a significant contribution which is dominant for sufficiently thin films. The study may be proven useful for the design and optimization of epitaxially grown electrical contacts.

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