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First Principles Study of Contact Resistance across Nickel-Treated-Graphene-MoS_2 Interfaces W.S. LEONG, Department of Electrical and Computer Engineering, National University of Singapore, Singapore 117583, X. LUO, Department of Physics and Graphene Research Centre, National University of Singapore, Singapore 117543, Y. LI, Department of Electrical and Computer Engineering, National University of Singapore, Singapore 117583, K.H. KHOO, S.Y. QUEK, Department of Physics and Graphene Research Centre, National University of Singapore, Singapore 117543, JOHN T.L. THONG, Department of Electrical and Computer Engineering, National University of Singapore, Singapore 117583 — Recently, Ni-treated-graphene electrodes were fabricated on MoS_2 using a dry transfer technique and metal-catalyzed graphene treatment process, yielding contact resistances as low as 200 $\Omega\mu$m and a substantial contact enhancement of $\sim$ 2 orders of magnitude relative to Ni-MoS_2 interfaces. By performing a Schottky barrier height (SBH) analysis on Ni-MoS_2 and Ni-graphene-MoS_2 interfaces using first-principles DFT calculations, we have found that the smaller contact resistance in Ni-treated-graphene-MoS_2 can be attributed to the smaller SBH of Ni-graphene-MoS_2 contacts. This reduction in SBH can in turn be related to the lower work function of Ni-graphene electrodes relative to Ni. The effect of Ni treatment further reduces the contact resistance due to stronger coupling between Ni and graphene edges.

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