Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

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 Ωμm 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.

K. H. Khoo
Department of Physics and Graphene Research Centre,
National University of Singapore, Singapore 117543

Date submitted: 14 Nov 2014
Electronic form version 1.4