

Abstract Submitted
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Graphene nanoelectronics from ab initio theory¹ JESSE MAASSEN, McGill University, WEI JI, HONG GUO — We employ atomic first principles theory to study the properties of realistic graphene nanoelectronic systems. We focus on the role of different contact materials and their effect on the transport properties at the graphene/metal junction. The current-voltage characteristics were calculated using density functional theory (DFT) combined with non-equilibrium Green's functions (NEGF).

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