# Charge transfer mechanism and breakdown of the Schottky-Mott limit of graphene/silicon van der Waals heterostructure

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**Abstract**: In this work, we present density functional theory calculations of the graphene/silicon (G/Si) van der Waals (vdW) interface. We showed that the charge transfer mechanism of the G/Si vdW interface is in terms of the metal-induced gap states theory but there is no Fermi level pinning due to the Fermi level shift in graphene. We also pointed out that, due to electrostatic screening property of the surface states of the Si substrate, the interfacial charge transfer may not lead to the evolution of a free-carrier depletion region in the subsurface region of the substrate. More interestingly, we revealed that the combination of the charge transfer potential and Fermi level shift in graphene can lead to a breakdown of the Schottky-Mott limit in the conventional metal/semiconductor interface model.

*Keywords*: graphene, semiconductor, van der Waals interface, Schottky-Mott limit, density functional theory