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Extraction of interlayer coupling and hopping potentials with misaligned hBN tunnel barriers in graphene/hBN/graphene tunnel FETs[1] AMITHRAJ VALSARAJ, LEONARD F. REGISTER, SANJAY K. BANERJEE, Univ of Texas, Austin — Reduction in interlayer tunneling due to weakened coupling across the rotationally misaligned interface between the channel layers and the tunnel barrier has been studied using atomistic density functional theory (DFT) simulations. The effects of rotational misalignment of the tunnel barrier layer between aligned channel layers was simulated with a prototypical graphene/hBN/graphene system. DFT simulation results suggest that the interlayer tunneling current for such heterostructures will be affected strongly by the rotational alignment of the hBN interface with respect to the graphene layers. We find that rotational misalignment between the channel layers and the tunnel barrier in this van der Waal's heterostructure can significantly reduce coupling between the channels by reducing, specifically, coupling across the interface between the channels and the tunnel barrier. Further, the hopping potentials for rotationally misaligned graphene/hBN/graphene were calculated using maximally localized Wannier functions technique, towards a better understanding of the source of reduced coupling.

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