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Development of a multi-space constrained density functional theory approach and its application to graphene-based vertical transistors[1]
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— We have been developing a multi-space-constrained density functional theory approach for the first-principles calculations of nano-scale junctions subjected to non-equilibrium conditions and charge transport through them [1,2]. In this presentation, we apply the method to vertically-stacked graphene/hexagonal boron nitride (hBN)/graphene Van der Waals heterostructures in the context of tunneling transistor applications. Bias-dependent changes in energy level alignment, wavefunction hybridization, and current are extracted. In particular, we compare quantum transport properties of single-layer (graphene) and infinite (graphite) electrode limits on the same ground, which is not possible within the traditional non-equilibrium Green function formalism. The effects of point defects within hBN on the current-voltage characteristics will be also discussed. [1] Kim, H. S. and Kim, Y.-H. Bulletin of the American Physical Society **60**, BAPS.2015.MAR.T23.15. [2] Kim, H. S. and Kim, Y.-H. Bulletin of the American Physical Society **61**, BAPS.2016.MAR.K31.5.

[1]Global Frontier Program (2013M3A6B1078881), Nano-Material Technology Development Programs (2016M3A7B4024133, 2016M3A7B4909944, and 2012M3A7B4049888), and Pioneer Program (2016M3C1A3906149) of the National Research Foundation

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