

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Study of local currents in 2D materials and junctions using a point source and TDDFT SHENGLAI HE, KALMAN VARGA, Vanderbilt University — The performance of nanoscale electronic device depends both on the property of junctions and conducting channels. An investigation of local electron pathway can help us better understand the relation between structure and transport property [1]. In this research, a combination of source potential and Time-Dependent Density Functional Theory is used to study local electron flow in heterogeneous material junctions and two-dimensional materials such as graphene and transition metal dichalcogenides. By injecting a conducting state at a single point and propagating the system in time, the wavefunction of the system in this specific state can be obtained. The local current can then be calculated from the wavefunction. \part\pard[1] Shenglai He, Arthur Russakoff, Yonghui Li, and Kalman Varga, . Appl. Phys. 120, 034304 (2016)

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Date submitted: 14 Nov 2016

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