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Chemically decorated line defect as a transport barrier in graphene[1] CARTER WHITE, Naval Research Laboratory, SMITHA VASUDEVAN, The George Washington University, DANIEL GUNLYCKE, Naval Research Laboratory — Graphene exhibits itinerant electrons propagating ballistically across its surface. To control electrons injected at a source contact, one needs transport barriers. With reliable transport barriers, electron flow could be directed and modified, a key requirement in nanoelectronics applications. In this presentation, we show that chemically decorated line defects in graphene could act as effective atomically-thin transport barriers. The considered 5-5-8 line defect has both been observed and controllably fabricated. Our density functional theory calculations indicate that diatomic hydrogen, oxygen, and fluorine react exothermically with the 5-5-8 defect inducing effective potentials along this line defect. Transport calculations show that these potentials reduce the electron transmission probability across the line defect converting it from semi-transparent to highly reflective to incoming electrons.

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