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Metal-Semiconductor Interfaces and Patterns in Functionalized Graphene ABHISHEK SINGH, EVGENI PENEV, BORIS YAKOBSON, Department of Mechanical Engineering and Materials Science, Rice University, Houston, TX 77006 — Functionalization offers a novel way to modify the electronic and magnetic properties of graphene. Specific topology is essential to achieve devices with the desired features. Using density functional theory, we demonstrate stability of several such configurations, (in single and double sided functionalized graphene) and analyze their electronic and magnetic properties. We show that "nanoroads" [1] and "nanodots" [2] of pristine graphene can be carved in the electrically insulating matrix of fully hydrogenated carbon sheet (graphane) [1]. Such one-dimensional roads display individual characteristics and, depending upon zigzag or armchair orientation, can be metallic or semiconducting. Furthermore, the wide enough zigzag roads become magnetic with energetically similar ferro- and antiferromagnetic states. Engineering magnetic, metallic, and semiconducting elements within the same mechanically intact sheet of graphene presents a new opportunity for applications. [1] A. K. Singh and B. I. Yakobson, Nano Lett., 9, 1540 (2009).

[2] A. K. Singh, E. S. Penev, and B. I. Yakobson submitted.

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