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Passivation and Depassivation of Defects in Graphene-based fieldeffect transistors¹ ANDREW O'HARA, Department of Physics and Astronomy, Vanderbilt University, PAN WANG, Department of Electrical Engineering and Computer Science, Vanderbilt University, CHRIS J. PERINI, School of Materials Science and Engineering, Georgia Institute of Technology, DANIEL M. FLEETWOOD, Department of Electrical Engineering and Computer Science, Vanderbilt University, ERIC M. VOGEL, School of Materials Science and Engineering, Georgia Institute of Technology, SOKRATES T. PANTELIDES, Department of Physics and Astronomy and Department of Electrical Engineering and Computer Science, Vanderbilt University — Field effect transistors based on graphene on amorphous SiO_2 substrates were fabricated, both with and without a top oxide passivation layer of Al_2O_3 . Initial I-V characteristics of these devices show that the Fermi energy occurs below the Dirac point in graphene (i.e. p-type behavior). Introduction of environmental stresses, e.g. baking the devices, causes a shift in the Fermi energy relative to the Dirac point. 1/f noise measurements indicate the presence of charge trapping defects. In order to find the origins of this behavior, we construct atomistic models of the substrate/graphene interface and the graphene/oxide passivation layer interface. Using density functional theory, we investigate the role that the introduction and removal of hydrogen and hydroxide passivants has on the electronic structure of the graphene layer as well as the relative energetics for these processes to occur in order to gain insights into the experimental results.

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