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Correlated Percolation Model of Graphene Hydrogenation ALEJANDRO SUAREZ, Department of Physics, Penn State University, TYLER MAUNU, School of Physics & Astronomy, University of Minnesota, JORGE O. SOFO, Department of Physics, Penn State University — Hydrogenation of graphene by exposure to an atomic hydrogen plasma is a random process. However, the presence of hydrogen already attached to the plane increases the sticking probability of incoming adatoms. We simulate this process as a correlated percolation model where the hydrogen occupation probability of a carbon site is increased or decreased depending on the hydrogenation of the nearest neighboring carbon atoms. This enhancement modifies the cluster distribution on the surface and consequently the electronic structure of the system. We study these effects with a tight binding model and find that, although the density of states at the Fermi level is greatly increased by hydrogenation, the inverse participation ratio shows that not all of these states will contribute to conduction. In fact, for hydrogenation levels of greater than 40% of the lattice, localized states begin to dominate at the Fermi level. A realistic set of values for the sticking probabilities is determined by analysis of the STM images of this system. Through the modeling of this mesoscopic process, we gain a better understanding of how chemically modified graphene is produced and what its transport properties are.

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