The role of long-range order and local sublattice symmetry breaking in defected graphene

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Previous work[1,2,3] has shown that certain periodic structural modifications on graphene can change graphene from a semimetal to a semiconductor without breaking A- and B-sublattice symmetry. However, there is still no understanding of such a mechanism based on fundamental considerations. We have developed a simple perturbative tight-binding model[4], which correctly predicts the analytic relation between bandgap opening and the supercell periodicity of the defected graphene without breaking the C_3 symmetry. Here, we generalize this model to investigate periodic defects violating the C_3 symmetry, employing a model Hamiltonian based on the virtual crystal approximation. In addition, non-Bravais superlattices are considered by including structure factors for each defect position in a unit cell. These predictions obtained from analytical modeling agree very well with first-principles electronic structure computations for partially H-passivated and BN doped graphene. This work was supported by DOE Early Career Award (No. DE-SC0006433).

[1] J. A. Furst, J. G. Pedersen, C. Flindt, N. A. Mortensen, M. Brandbyge, T. G. Pedersen, and A.-P. Jauho, New J. of Phys. **11**, 095020 (2009).

[2] R. Zhao, J.Wang, M. Yang, Z. Liu, and Z. Liu, J. Phys. Chem. C **116**, 21098 (2012).

[3] W. Oswald and Z. Wu, Phys. Rev. B **85**, 115431 (2012).

[4] M. Dvorak and Z. Wu, submitted to Scientific Reports.