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First-principles and Tight-binding Investigations of Graphene-like Systems[1] X.W. SHA, E.N. ECONOMOU, D.A. PAPACONSTANTOPOULOS, George Mason University, M. PEDERSON, M.J. MEHL, Naval Research Laboratory, M. KAFESAKI, University of Crete — We have performed first-principles calculations of graphene-like systems with large unit cells of the order of 100 atoms. These are mostly quasi-circular pieces of graphene with or without hydrogen atoms to passivate dangling bonds. We have also introduced nitrogen replacements of carbon atoms to explore possibilities of creating a quantum-mechanical analog of the split-ring resonator used in negative refractive index metamaterials. In addition, vibrational spectra were calculated to check the stability of the small flakes. Furthermore, we have used the NRLMOL DFT code with extensions to treat an AC magnetic field coupled to spin and orbital moments. We simulate the graphene-like system to a circuit model to show the cancellation of individual loop currents and the emergence of an edge ballistic current. A tight-binding Hamiltonian was fitted to our NRLMOL results using the NRLTB method. The TB approach starts with an exact fit to the benzene molecule and the resulting TB parameters are transferable to the larger molecules matching well the HOMO-LUMO gap found by the DFT. The NRLTB scheme allows to calculate the electronic spectra of much bigger systems, and examples with results for systems with more than a thousand atoms will be presented.

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