Large-Scale Self-Consistent Simulation of Multilayered Graphene Devices
DENIS ARESHKIN, BRANISLAV K. NIKOVIĆ, University of Delaware — We use the Density Functional Theory-based Self-Consistent Environment-Dependent Tight-Binding (SC-EDTB) and self-consistent Non-equilibrium Green function formalism (NEGF) to test the all-graphene multilayer circuit concept. The key element of multi-layered circuits, which are expected to become available through press-print technology, is the heavily perforated graphene layer. The latter serves as an electrical insulator due to its relatively large band gap, and poor ballistic coupling to the conductive parts of the circuit. High bias $I - V$ characteristics for various normally-ON and normally-OFF transistor configurations were simulated, and transistor tolerance to manufacturing defects and imperfections was tested. The usage of SC-EDTB-NEGF makes it possible to model quantum transport through realistic devices composed of large number of carbon atoms ($\sim 10000$), which are within the reach of presently available processing techniques. Other circuit elements, such as electric interconnects between different layers, wire crossings, and electric interconnects within the same layer are also considered.