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Numerical simulation of time-dependent transport in graphene DHARMENDAR REDDY, PRIYAMVADA JADAUN, LEONARD F. REGISTER, SANJAY K. BANERJEE, The University of Texas at Austin — We present a numerical method for modeling time-dependent quantum transport in graphene. The time-dependent Schrodinger equation is solved with a pi-orbital-based atomistic tight-binding Hamiltonian. A novel variation of an alternating-direction semi-implicit scheme is employed on the hexagonal tight-binding lattice to maintain stability and conserve probability while achieving computational efficiency. Open boundaries including source terms to allow time-dependent non-equilibrium Green's function (NEGF) calculation of graphene devices will be discussed.

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