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A multiphysics numerical technique for THz-frequency carrier transport in semiconductors and metals¹ K. J. WILLIS, S. C. HAGNESS, I. KNEZEVIC, University of Wisconsin - Madison — We present a novel computational tool for THz-frequency characterization of materials with high carrier densities, such as highly-doped semiconductors and metals. The numerical technique tracks carrier-field dynamics by combining, for the first time, the ensemble Monte Carlo (EMC) simulator of carrier dynamics with the finite-difference time-domain (FDTD) technique for Maxwell's equations and the molecular dynamics (MD) technique for close-range Coulomb interactions. While EMC/FDTD has been proven to accurately characterize high-frequency behavior in electronic systems with low carrier densities ($<10^{16}$ cm⁻³), the inclusion of short-range Coulomb interactions via MD becomes necessary at higher carrier densities ($>10^{18}$ cm⁻³). This three-pronged multiphysics technique captures electromagnetic wave propagation and transport in materials in which carrier dynamics may be strongly impacted by Coulomb interaction between carriers.

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