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Circuit elements at optical frequencies: A synthesis of first principles electronic structure and circuit theories C. TANG, R. RAMPRASAD, Department of Materials Science and Engineering, University of Connecticut — We present a new first principles based method to determine the equivalent circuit representations of nanostructured physical systems at optical frequencies. This method involves the determination of the frequency dependent effective permittivity of two constructs: an ordered composite system consisting of physical nano-elements using density functional theory, and an ordered arrangement of impedances using transmission line theory. Matching the calculated effective permittivity functions of these two constructs has enabled a mapping of the physical nano-system to its equivalent circuit. Specifically, we will show that silicon nanowires and carbon nanotubes can be represented as a series combination of inductance, capacitance and resistance. Once this mapping has been reasonably accomplished for a variety of physical systems, the nano-elements can be combined suitably to result in equivalent circuit topologies appropriate for optical and nanoelectronic devices, including left-handed (or negative refractive index) materials.

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