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# Simulation Design for Photovoltaics Using Finite Difference Time Domain and Quadratic Complex Rational Function Methods

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## ABSTRACT

Photovoltaics (PV) can in principle supply enough renewable energy to offset a great deal of fossil fuel usage. To achieve this transition, it is critical to develop improved PV cells with decreased material costs and improved efficiencies. This goal can be greatly facilitated by a tool simulating the absorption and efficiency of experimentally relevant 3-D PV designs made of realistic materials, including those that have not yet been discovered. By incorporating the quadratic complex rational function algorithm (QCRF) with the finite difference time domain methods (FDTD), simulations can include frequency response and optical properties, while allowing full customization of tandem or single junction photovoltaic cell designs. FDTD models how electro-magnetic waves travel through materials and vacuum, while QCRF allows for more realistic material dispersion. This tool allows users to easily incorporate commonly-used photovoltaic materials. By incorporating the QCRF-FDTD method, the simulation provides increased material & design customization with a shorter runtime than most current tools. nanoHUB.org—an open-access science gateway for cloud-based simulation tools and resources in nanoscale science and technology. This tool will predict PV absorption spectra, external quantum efficiencies, short-circuit currents, and power conversion efficiencies, to help guide future experiments toward higher efficiencies and lower costs.

## KEYWORDS

photovoltaic, finite, difference, time, domain, quadratic, complex, rational, function, simulation