Summit to: Computational Material Science

Monte Carlo methods in computational materials science

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EXTENDED ABSTRACT: Monte Carlo (MC) methods in computational materials science are a powerful simulation tool for studying material properties and physical processes. The MC methods have a wide range of applications, from phase transitions in materials [1], materials design [2], to electronic structure calculations [3]. Here, we present a brief overview of recent developments in this topic, focusing on using MC simulations for material characterization.

Keywords: Monte Carlo simulations; computational materials science.

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BIOGRAPHY

Hieu T. Nguyen-Truong earned PhD in 2015 from Volgograd State Technical University, Russia. He is interested in electron scattering and dielectric properties of materials. His studies focus to the fields of applied physics and materials science.