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Mathematical Numerical Simulations in Chemical Physics

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Message from the Guest Editor

Mathematical numerical simulations are a convergence of computer science, mathematics, physics, chemistry, and sometimes materials science. It is at the interface between these disciplines where most exciting new developments in the field of numerical simulation are being made. Using mathematical numerical simulations in chemical physics allows a significant reduction in the molecular and material costs associated with production. However, it is imperative for a chemical physicist to use correct numerical simulation approaches in modeling. Considering the current level of advanced mathematical numerical simulations, this Special Issue illuminates how chemical physicists should properly define the chemical and physical problem statement, choose the mathematical numerical simulation approach, and use computer and software applications during the solution of a particular problem. This Special Issue aims to focus the chemical physics community's attention on the bridge that exists between mathematical numerical simulations and other related fields of chemical physics.

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Message from the Editor-in-Chief

The journal *Mathematics* publishes high-quality, refereed papers that treat both pure and applied mathematics. The journal highlights articles devoted to the mathematical treatment of questions arising in physics, chemistry, biology, statistics, finance, computer science, engineering and sociology, particularly those that stress analytical/algebraic aspects and novel problems and their solutions. One of the missions of the journal is to serve mathematicians and scientists through the prompt publication of significant advances in any branch of science and technology, and to provide a forum for the discussion of new scientific developments.

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