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# Special Issue on Computational Chemistry

## Call for Papers

Computational chemistry has its roots in the early attempts by theoretical physicists, beginning in 1928, to solve the Schrödinger equation using hand-cranked calculating machines. These calculations verified that solutions to the Schrödinger equation quantitatively reproduced experimentally observed features of simple systems such as the helium atom and the hydrogen molecule. The goal of this special issue is to provide a platform for scientists and academicians all over the world to promote, share, and discuss various new issues and developments in the area of **Computational Chemistry**.

In this special issue, we invite front-line researchers and authors to submit original research and review articles that explore **Computational Chemistry**. In this special issue, potential topics include, but are not limited to:

- Quantum-mechanical methodologies for energy and electron transport
- Non-equilibrium statistical mechanics
- Theoretical and computational approaches for biomolecular simulations
- Computational modeling of heterogeneous chemistry relevant to climate and the environment
- Electronic structure calculations of organic, inorganic and organometallic complexes,
- Molecular mechanics
- Molecular dynamics
- Chemical Kinetics and Molecular Reaction Dynamics

Authors should read over the journal's For Authors carefully before submission. Prospective authors should submit an electronic copy of their complete manuscript through the journal's Paper Submission System.

Please kindly specify the "**Special Issue**" under your manuscript title. The research field "**Special Issue - *Computational Chemistry***" should be selected during your submission.

Special Issue timetable:

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|---|---|
| Submission Deadline | June 24th 2022 |
| Publication Date | August 2022 |

**Guest Editor:**


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