

## Special Issue

# Advances in Computational Software for Chemistry and Materials Science

### Message from the Guest Editors

This Special Issue discusses the latest software developments in computational chemistry, biomolecular simulation, and materials science. Building these tools is challenging due to the need for massive parallelization and handling data- and computation-intensive tasks.

However, recent advances are making it possible to tackle complex problems more efficiently, helping researchers model molecular interactions, study chemical reactions, and design new materials. This Special Issue highlights innovative solutions that improve performance, usability, and accuracy, driving progress in scientific research and industry applications.

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### Deadline for manuscript submissions

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