

## Special Issue

# Advances in Computer Simulation of Condensed Matter Systems

### Message from the Guest Editor

Progress in computational capabilities is driving condensed matter research to new levels, not only due to the continuously improving processing technology, but also due to the advancements and widespread use of machine learning (ML) and artificial intelligence (AI) in research. Examples include drug design, adsorption studies in porous materials, analysis of the effects of mutations on protein structure and function, design of materials for colloidal systems, discovery of novel polymeric materials, and forcefield development. This Special Issue on “Advances in Computer Simulation of Condensed Matter Systems” will focus on computational works that present novel advances in simulations of condensed matter systems. Submissions to this Special Issue may include but are not limited to the following topics:

- Drug discovery, and biomolecular structure and dynamics (proteins, lipids, nucleic acids);
- Colloidal systems, polymers, and nanomaterials;
- Porous material structure and adsorption;
- Interfacial and surface phenomena;
- Supramolecular assemblies—structure and transport phenomena.

### Guest Editor

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### Deadline for manuscript submissions

15 August 2025



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