

## Special Issue

# Molecular Dynamics, Numerical Simulation and Integrated Method to Study Materials Processing and Manufacturing

### Message from the Guest Editors

This Special Issue focuses on advancements in both individual and integrated simulation techniques, addressing topics like the study of phase transitions, defect dynamics, microstructure evolution and material property predictions under extreme conditions. Additionally, this issue explores the synergy between molecular dynamics simulations, continuum models, finite element methods and other computational tools, highlighting the value of these integrated approaches in developing a more complete understanding of materials behavior in real-world manufacturing environments. In this Special Issue, original research articles and reviews are welcome. Topics of interest include, but are not limited to, the following research areas:

- Atomistic and mesoscale modeling;
- Computational materials science;
- Advanced manufacturing simulations;
- Tribology and surface engineering;
- Metal forming and machining;
- Polymer and composite material processing;
- Heat treatment and phase transformations;
- Nanomaterials and nanomanufacturing.

### Guest Editors

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### Deadline for manuscript submissions

30 November 2025



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