



## Molecular Modeling for Industrial Process Design

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Deadline for manuscript  
submissions:

**closed (31 March 2022)**

### Message from the Guest Editors

In this Special Issue entitled “Molecular Modeling for Industrial Process Design”, we will highlight and celebrate the latest research in the application of molecular modeling for process design applications. Topics include, but are not limited to:

- Molecular thermodynamic models for process modeling, simulation, optimization, and control: equations of state, excess Gibbs free energy models, and related methods;
- Molecular-based property prediction for early stage process development and design: molecular simulation, electronic structure calculations, group-contribution methods, and related methods;
- Molecular-based prediction of reaction mechanisms and rate expressions;
- Molecular models for process intensification;
- Use of molecular modeling to better understand existing process technologies.

We welcome contributions in the form of full-length articles, short communications, and reviews.





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## Message from the Editor-in-Chief

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