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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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Special Issue

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Message from the Editor-in-Chief

Processes (ISSN 2227-9717) provides an advanced forum for process/system-related research in chemistry, biology, material, energy, environment, food, pharmaceutical, manufacturing and allied engineering fields. The journal publishes regular research papers, communications, letters, short notes and reviews. Our aim is to encourage researchers to publish their experimental, theoretical and computational results in as much detail as necessary. There is no restriction on paper length or number of figures and tables.

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