Special Issue

Molecular Modeling for Industrial Process Design

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.

Guest Editors

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Deadline for manuscript submissions

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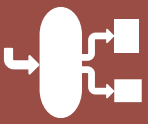

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Message from the Editor-in-Chief

You are invited to contribute either a research article or a comprehensive review for consideration and publication in *Processes* (ISSN 2227-9717). *Processes* is published in open access format – research articles, reviews, and other content are released on the internet immediately after acceptance. The scientific community and the general public have unlimited, free access to the content. As an open access journal, *Processes* is supported by the authors and their institutes through the payment of article processing charges (APCs) for accepted papers. We would be pleased to welcome you as one of our authors.

Editor-in-Chief

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