Special Issue

Modeling and Optimization for Green Energy Materials: Machine Learning, Conventional, and Hybrid Approaches

Message from the Guest Editors

This Special Issue, "Modeling and Optimization for Green Energy Materials: Machine Learning, Conventional, and Hybrid Approaches", aims to compile research that integrates mechanistic simulation methods, machine learning, and hybrid strategies to study energy materials. Topics of interest include, but are not limited to, the following:

- Modeling, process simulation, and optimization to produce green energy materials using conventional or hybrid approaches.
- Applications of machine learning and artificial intelligence in the design, prediction, and control of sustainable materials and processes.
- The integration of digital tools and application of process simulators and data-driven models to enhance energy efficiency and material performance.
- Techno-economic, environmental, and life-cycle assessments supported by simulation and intelligent modeling techniques.

We welcome original contributions, both experimental and computational, that advance the state of the art of materials science, process engineering, and data science regarding the energy transition.

Guest Editors

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Editor-in-Chief

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