Special Issue

Editorial Board Members' Collection Series: Molecular Simulation and Thermodynamics

Message from the Guest Editors

This Special Issue is devoted to multiscale materials modelling approaches for the design of safe, sustainable and functional materials and their use for various applications. In fact, research considering atomistic- and molecular-level simulations, such as first-principles (specially Density Functional Theory) and classical molecular dynamics simulations for predicting a materials' relevant physicochemical properties and phase equilibria in solid, liquid and gas phases, are welcome. Mesoscale simulations as well as upscale theoretical studies (including computational fluid dynamics, process engineering) coupling molecular level simulations with thermodynamics modelling (including advanced equations of state) will be also considered. Studies coupling fundamental atomic-level simulations with thermodynamics modelling and process engineering are additionally welcome. Finally, in silico studies for predicting materials' safety and sustainability as well as their environmental impact will be also included in this Special Issue.

Guest Editors

Prof. Dr. Santiago Aparicio

Prof. Dr. Johan Jacquemin

Prof. Dr. Steve Lustig

Dr. Andrew S. Paluch

Prof. Dr. William E. Acree, Jr.

Deadline for manuscript submissions

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Thermo
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
thermo@mdpi.com

mdpi.com/journal/thermo

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About the Journal

Message from the Editor-in-Chief

Thermo (ISSN: 2673-7264) is an international, peer-reviewed, and open access journal that publishes original research papers, reviews, and Special Issues dealing with experimental, theoretical, and applied thermal sciences. Both theoretical (simulation) and/or experimental research papers within our journal's scope are of particular interest, including satellite-related topics considering thermophysics, solubility phenomena, chemical thermodynamics, and chemical engineering. We encourage scientists to publish their results in as much detail as possible, and there is no restriction on the maximum length of papers. We greatly appreciate suggestions for enhancing the journal.

Editor-in-Chief

Prof. Dr. Johan Jacquemin
Materials Science, Energy, and Nano-Engineering MSN Department, Mohammed VI Polytechnic University, Lot 660, Hay Moulay Rachid, Ben Guerir 43150, Morocco

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