thermo

an Open Access Journal by MDPI

Tracked for Impact Factor

CITESCORE 2.1

# Editorial Board Members' Collection Series: Molecular Simulation and Thermodynamics

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:
**closed (31 March 2024)**

## 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.