10th Anniversary of *Computation*—Computational Chemistry

Guest Editors:

Prof. Dr. Karlheinz Schwarz
Theoretical Chemistry Group, Materials Chemistry, TU Wien, A-1060 Vienna, Austria

Prof. Dr. Henry Chermette
Institut des Sciences Analytiques, Université de Lyon, UMR 5280, CNRS, Université Lyon 1 - 5, rue de la Doua, F-69100 Villeurbanne, France

Deadline for manuscript submissions:
closed (30 November 2023)

Message from the Guest Editors

Computational chemistry is crucial for understanding the relationship between atomic structure and material properties. Many papers, including in this journal, have been published on this topic. Simulations often simplify computations through idealizations. Methodology analysis is critical for enhancing computation quality, particularly for electronic structure using density functional theory (DFT) based on functionals. Determining which functionals align with experimental data is crucial. Additional important factors include temperature, pressure, magnetism, substitutions, and relativistic effects (for heavy elements). Accuracy is essential for evaluating similar cases like magnetic anisotropy. Improving efficiency enables exploration of complex structures representing real systems. Systematic studies unveil trends, enhancing structure-property relations with new insights. We plan to publish a Special Issue addressing current challenges and future innovations. Solid-state research, numerical analysis, machine learning, AI, computational biology, and bioinformatics are also significant in computational chemistry.

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Special Issue

Editor-in-Chief

Prof. Dr. Ali Cemal Benim
Center of Flow Simulation (CFS),
Department of Mechanical and
Process Engineering, Duesseldorf
University of Applied Sciences, D-
40476 Duesseldorf, Germany

Message from the Editor-in-Chief

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The editorial board and staff of *Computation* are dedicated to establishing a benchmark journal for the world scientific and engineering communities for original research articles, reviews, conference proceedings (i.e., peer reviewed full articles), and communications, in the cutting-edge areas of computational biology, computational chemistry, and computation in engineering.

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