Special Issue

Advances in Computational Chemistry for the Molecule/Material Design and Chemical Process Applications

Message from the Guest Editors

Computational chemistry is increasingly merging with all the other branches of chemistry, providing information essential for interpreting experimental findings, predicting the properties of new molecules, designing new substances and materials with desired properties, and designing new chemical processes. The theoretical models and the computational approaches are continuously being refined to better respond to new tasks stemming from ever-growing research and from practical challenges. This continuously broadens the scope of computational chemistry. Applications encompass areas such as drug design, computer-aided molecular design, designing new substances and mechanisms to make chemical production cleaner, designing materials for efficient energy storage, etc. This Special Issue will highlight this continuous progress and scope expansion, ranging from those associated with theories and models to the many applications of the study of molecules and materials. It, thus, will provide experts and students with an overview of what computational chemistry can do in its current state, as well as perspectives on and potential for further developments in the near future.

Guest Editors

Prof. Dr. Liliana Mammino

Department of Chemistry, University of Venda, Thohoyandou 0950, South Africa

Prof. Dr. Federico Palazzetti

Dipartimento di Promozione delle Scienze Umane e della Qualità della Vita, Università Telematica San Raffaele, 00166 Roma, Italy

Deadline for manuscript submissions

31 December 2025

Processes

an Open Access Journal by MDPI

Impact Factor 2.8
CiteScore 5.5

mdpi.com/si/241935

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

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Editor-in-Chief

Prof. Dr. Giancarlo Cravotto
Department of Drug Science and Technology, University of Turin, Via P. Giuria 9, 10125 Turin, Italy

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