

## Special Issue

# Selected Papers Associated with the Modeling and Design of Molecular Materials (MDMM 2022) Conference

### Message from the Guest Editors

The Modeling and Design of Molecular Materials 2022 (MDMM 2022) conference is an interdisciplinary meeting devoted to the various aspects of conceiving materials with predefined properties. The key term is “molecular material”, which in the context of the conference means drugs and drug carriers (focused on cancer), catalysts, with an emphasis on photocatalysis (e.g., solar energy conversion) or theozymes (theoretically designed biocatalysts), materials for hydrogen storage (green fuel), conductive polymers (e.g., electronics, biosensors), etc. Nowadays, computer modeling seems to be a crucial step for the rational design of materials with demanded properties. Thus, during this prospective event we hope to gather specialists who develop computational methods useful in the computer-aided design of materials as well as those who employ molecular modeling at the very early stages of their projects and for whom a computational approach eventually leads to practical solutions.

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### Guest Editors

Prof. Dr. Janusz Rak

Dr. Lidia Chomicz-Mańka

Dr. Magdalena Zdrowowicz

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### Deadline for manuscript submissions

closed (30 April 2023)



## International Journal of Molecular Sciences

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The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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### Editor-in-Chief

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