Special Issue

NMR Spectroscopy in Materials Chemistry

Message from the Guest Editors

Chemical shifts and spin-spin coupling constants observed by NMR spectroscopy are very sensitive to the valence and core electronic structures of molecules and represent an indispensable strategic tool of their structural elucidation. Nowadays, it is rare that modern synthetic work can do without the combination of the state-of-the-art homo- and heteronuclear NMR techniques with high-quality quantum chemical calculations. This especially concerns synthesis of novel compounds containing heavy elements, for which there may occur mis-assignments of NMR signals. In this sense, the development of new computational approaches, relativistic or not, to the NMR parameters that are intended to increase the accuracy of NMR spectra simulation is of paramount importance for today. This Special Issue entitled "NMR Spectroscopy in Materials Chemistry" will provide researchers with the opportunity to publish their most recent discoveries in the field of high-quality experimental NMR studies of organic and inorganic compounds as well as the theoretical studies of the NMR spectral parameters. Dr. Irina L. Rusakova

Guest Editors

Dr. Irina Rusakova

A.E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of Sciences, Favorsky St. 1, 664033 Irkutsk, Russia

Dr. Lyudmila I. Larina

A.E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of Sciences, Favorsky St. 1, 664033 Irkutsk, Russia

Deadline for manuscript submissions

closed (20 January 2025)



International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9 CiteScore 9.0 Indexed in PubMed



mdpi.com/si/153699

International Journal of Molecular Sciences Editorial Office MDPI, Grosspeteranlage 5 4052 Basel, Switzerland Tel: +41 61 683 77 34 ijms@mdpi.com

mdpi.com/journal/ ijms





International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9 CiteScore 9.0 Indexed in PubMed





Message from the Editor-in-Chief

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.

Editor-in-Chief

Prof. Dr. Maurizio Battino

Department of Odontostomatologic and Specialized Clinical Sciences, Sez-Biochimica, Faculty of Medicine, Università Politecnica delle Marche, Via Ranieri 65, 60100 Ancona, Italy

Author Benefits

Open Access:

free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, PMC, MEDLINE, Embase, CAPlus / SciFinder, and other databases.

Journal Rank:

JCR - Q1 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

