Special Issue

Molecular Structure and Dynamics Probed by Spectroscopic Techniques and Computational Approaches: New Trends by NMR, FTIR, Neutron Scattering and Simulation

Message from the Guest Editors

Spectroscopic techniques such as Nuclear Magnetic Resonance (NMR), Fourier Transform Infrared (FTIR) spectroscopy, and neutron scattering are among the most powerful experimental methods for probing the molecular structure and dynamics of a wide variety of systems. Therefore, these techniques are used in many areas of science including physics, chemistry, medicine, food science, and cultural heritage. The corresponding results can serve as a benchmark and guide for the many models that are being developed with the aim of developing detailed “analytical” insights about the properties of the studied systems. This Special Issue aims to highlight new advances in the application of the mentioned spectroscopic techniques and computational approaches for the study of molecular structure and dynamics of those systems that are particularly interesting within physical chemistry and its related fields. Special emphasis will be given to innovative methodologies applied at the molecular level and to results with broad scientific relevance.

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Deadline for manuscript submissions

closed (31 December 2020)

International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed

mdpi.com/si/33701

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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