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

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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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Message from the Editor-in-Chief

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