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Research on Molecular Dynamics

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Message from the Guest Editors

Dear Colleagues,

Molecular dynamics (MD) simulation has emerged as a fundamental research methodology in biology, material sciences, and chemical physics. Many advanced tools, including cryo-electron microscopy, X-ray crystallography, solid-state nuclear magnetic resonance, and fiber diffraction, have been developed to determine molecular structure and function. Recent advances in the computational platform, algorithms, analysis tools, software, and high-performance computing have made molecular simulations useful for investigating more complicated and large systems.

We warmly welcome your contributions to this Special Issue on "Research on Molecular Dynamics." This Special Issue will cover any aspect of MD simulation, including the theory, techniques, and computational or methodological developments for the result analysis. Original research papers and review articles addressing MD simulation applications to diverse biomolecular systems, interactions, and functions are welcome. Submission of combined simulation and experimental studies is also encouraged.

Prof. Dr. II Soo Moon Dr. Raju Dash Guest Editors













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Message from the Editor-in-Chief

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