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Editorial

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Preface

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With the completion of Volume 2, Molecular Modeling Connect proudly marks its second year of contributions to the scientific community, representing another significant step forward in its mission to serve as a dynamic forum for the global molecular modeling community. This volume stands as a testament to the growing relevance of computational and theoretical approaches in shaping modern molecular science and to the enthusiasm of researchers who are advancing this field through innovation and collaboration.

The articles published in Volume 2 showcase the expanding influence of molecular modeling across chemistry, biology, materials science, and interdisciplinary research. They highlight how computational techniques have evolved from being merely auxiliary tools to essential drivers of innovation, enabling the prediction of molecular behavior, the rational design of molecules and materials, and the exploration of systems beyond the reach of traditional experimental methods. Together, these contributions reflect the creativity and technical excellence of a community that is redefining how molecular-level problems are approached and solved.

At Molecular Modeling Connect, we believe that scientific progress thrives on connections between disciplines, between theory and experiment, and among researchers at different stages of their careers. The diversity of contributions in this volume exemplifies this vision, bringing together varied perspectives and methodologies that collectively advance molecular modeling as a unifying language of molecular science. Our goal is not only to disseminate high-quality research but also to encourage dialogue, collaboration, and the generation of new ideas that transcend traditional disciplinary boundaries.

I extend my sincere appreciation to the authors who have chosen Molecular Modeling Connect as the home for their work, and to the reviewers whose thoughtful and rigorous evaluations uphold the journal's scientific integrity. Their combined efforts ensure that every published article makes a meaningful contribution to the field's advancement. I also thank the editorial team and our publisher, SCIFINITI Publishing, for their continued dedication to building a journal that is both accessible and impactful.

As we close Volume 2, we do so with confidence in the future of Molecular Modeling Connect. We invite researchers from around the world to contribute to upcoming volumes by submitting their most innovative and forward-looking work in molecular modeling, simulation, and data-driven molecular science. We aspire for this journal to continue to grow as a recognized platform for high-quality research and a source of inspiration for scientists exploring the molecular world through computational methods.

On behalf of the editorial board, I extend my gratitude to our readers and contributors for being part of this journey. We look forward to the discoveries and innovations that future volumes will showcase.

Dr. Robert Vianello
Editor-in-Chief
Molecular Modeling Connect

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