frontiers | Frontiers in Physics

TYPE Editorial
PUBLISHED 29 July 2025
DOI 10.3389/fphy.2025.1662523

OPEN ACCESS

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RECEIVED 09 July 2025
ACCEPTED 21 July 2025
PUBLISHED 29 July 2025

CITATION
Khalilov U, Berdiyorov GR, Zhang Y and Yusupov M (2025) Editorial: Advancing understanding of biological and nanostructured materials through atomistic simulations.
Front. Phys. 13:1662523.
doi: 10.3389/fphy.2025.1662523

Editorial: Advancing understanding of biological and nanostructured materials through atomistic simulations

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KEYWORDS

atomistic simulations, molecular dynamics (MD), nanostructured materials, biological materials, free energy calculations, oxidative stress, topological indices

Editorial on the Research Topic
Advancing understanding of biological and nanostructured materials through atomistic simulations

Atomistic simulations have become a cornerstone in the interdisciplinary fields of materials science, biophysics, and chemistry. These powerful computational methods offer unprecedented insights into the atomic-scale behavior of complex systems. Despite significant progress, a gap often remains between theoretical predictions and experimental observations. Unanswered questions persist regarding the intricate mechanisms of biological processes and the targeted synthesis of novel nanostructures with desired properties.

It was to address these challenges that we launched the Research Topic, *Advancing Understanding of Biological and Nanostructured Materials through Atomistic Simulations*. The aim was to harness the power of simulation to explore fundamental scientific questions and bridge the gap between theory and experiment. In line with this objective, the Research Topic of articles presented here directly addresses key themes outlined in our original call, including the effects of plasma on biomolecules, the synthesis pathways of materials, and the properties of novel 2D nanostructures.

Providing a crucial methodological framework for this field, Fu et al. offer a comprehensive mini-review of free energy calculation methods. The authors categorize and analyze a suite of powerful techniques (including endpoint methods like molecular mechanics Poisson-Boltzmann surface area (MM/PBSA), alchemical methods such as free energy perturbation (FEP) and thermodynamic integration (TI), and pathway methods like Umbrella Sampling) and discuss their advantages and limitations specifically for biomolecule-nanomaterial systems. This work serves as an essential guide for researchers navigating the complexities of accurately quantifying molecular interactions.

Demonstrating the power of these techniques to address neurodegenerative disease, Akramov et al. employed extensive molecular dynamics simulations and Potential of Mean Force (PMF) calculations to investigate how oxidation affects the stability of α-synuclein fibrils, a pathological hallmark of Parkinson's disease. Their research provides a detailed molecular picture of how oxidative modifications disrupt key salt bridges and hydrophobic packing, leading to a significant reduction in fibril stability and a lower dissociation free energy. These findings reinforce the critical role of oxidative stress in modulating fibril dynamics.

In a similarly impactful biomedical application, Tan et al. utilized reactive molecular dynamics (ReaxFF-MD), a technique capable of modeling bond-breaking and formation, to elucidate the cleavage mechanism of the SARS-CoV-2 spike protein by plasma-generated reactive oxygen and nitrogen species (RONS). By simulating chemical bond breaking, their study identified specific RONS, such as $^1O_2$ and HOONO, as being particularly potent in destroying the protein's integrity. The work highlights the synergistic effect of different RONS and provides a mechanistic basis for the antiviral potential of cold atmospheric plasma.

The scope of the Research Topic also extends to the rational design of inorganic nanomaterials. In a combined computational and experimental study, Li et al. investigated how the molecular structure of various carboxylic acids influences the crystal morphology and mechanical strength of α-hemihydrate gypsum. Their molecular dynamics simulations successfully predicted how factors like the number and spacing of carboxyl groups affect crystal growth, establishing screening principles that were experimentally validated to produce gypsum with superior mechanical properties.

Complementing these simulation-based approaches, Hakeem et al. offered a theoretical perspective on predicting material properties. They applied graph theory to derive reverse degree-based topological indices for γ-graphyne, a novel carbon allotrope with exceptional electronic potential. By developing closed-form mathematical formulas for these molecular descriptors, their work provides a powerful, high-throughput method to predict the physicochemical properties of new materials, guiding future synthesis and experimentation often without the computational expense of full atomistic simulations.

Taken together, these articles paint a compelling picture of a dynamic and rapidly advancing field. They showcase a remarkable range of computational tools applied to an equally diverse set of scientific problems. The common thread is the generation of atomic-level insights that are pivotal for progress.

Looking forward, the integration of machine learning with traditional physics-based simulations promises to push the boundaries even further. We hope that the work presented in this Research Topic will serve as a valuable resource and inspire further research into the fascinating atomic landscapes of biological and nanostructured materials.

Finally, we wish to extend our sincere gratitude to all the authors who contributed their excellent work to this Research Topic. We are also deeply grateful to the reviewers whose diligent efforts were instrumental in upholding the high quality of the publications and to the Frontiers editorial team for their invaluable support throughout the process.

Author contributions

UK: Writing – original draft. GB: Writing – review and editing. YZ: Writing – review and editing. MY: Writing – review and editing.

Funding

The author(s) declare that no financial support was received for the research and/or publication of this article.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

The author(s) declared that they were an editorial board member of Frontiers, at the time of submission. This had no impact on the peer review process and the final decision.

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The author(s) declare that Generative AI was used in the creation of this manuscript. Editing and Polishing: To revise the manuscript for clarity, style, and tone throughout the preparation process.

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