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Molecular Simulations of Energy Materials

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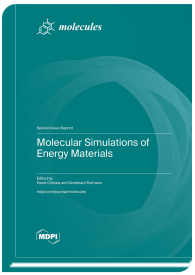

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The continuous rise in global energy demand, together with the depletion of conventional resources, places increasing pressure on the scientific community to develop materials that enable clean, efficient, and sustainable energy generation, storage, and utilization. The phenomena underlying these processes are inherently complex, often occurring simultaneously across multiple spatial (from atomic to macroscopic) and temporal (from femtoseconds to years) scales. While experimental investigations remain fundamental to the study of energy and environmental systems, our understanding of material behavior under extreme conditions—particularly at the microscopic level—remains limited. Computational molecular science has therefore become an indispensable complement, offering powerful tools to analyze and describe the mechanisms governing these phenomena.

Molecular simulations, including static calculations, Molecular Dynamics, and Monte Carlo methods, rely on intra- and intermolecular forces determined at quantum, classical, or coarse-grained levels. These approaches provide essential insights into the structure and dynamics of energy materials and help interpret experimental data. The integration of particle-based and continuum methods within multiscale frameworks further enhances our ability to capture the hierarchical nature of processes in energy and environmental materials. Collectively, these computational methodologies form a vital foundation for understanding, predicting, and optimizing the behavior of energy materials.

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