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MOLECULAR SIMULATION FOR DESIGNING CHEMICAL REACTIONS: APPLICATION OF COMPUTATIONAL CHEMISTRY METHODS IN UNDERSTANDING REACTION MECHANISMS AND MOLECULAR DESIGN

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Abstract

Molecular simulation, a cornerstone of computational chemistry, has revolutionized the understanding and design of chemical reactions. This study explores the application of computational chemistry methods in elucidating reaction mechanisms and guiding molecular design. Employing diverse algorithms rooted in classical and quantum mechanics, molecular simulations unravel the dynamic behavior of molecules, offering insights into spatial arrangements and temporal evolution. A comparative analysis of simulation algorithms reveals their mathematical foundations, exemplary applications, and computational costs. Standard computational modeling methods, including Density Functional Theory and molecular mechanics, strike a balance between accuracy and efficiency. Case studies demonstrate the efficacy of molecular dynamics and quantum mechanics calculations in dissecting enzymatic, organic, and gas-phase reactions. Computational methods contribute to predicting reaction pathways and mechanisms, accelerating the discovery of novel reactions. In molecular design, simulations guide conformational analysis and electronic structure predictions, culminating in successful drug discovery, materials science, and catalysis outcomes. Challenges, opportunities, and practical applications in research and industry are discussed. This study underscores the transformative role of

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