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Molecular Dynamics and Catalysis

Lobaina Alrhia

Department of Fluid Mechanics, University of Milan, Milan, Italy

Introduction

Molecular dynamics (MD) is a computer simulation method for studying atoms and molecules' physical motions. The atoms and molecules are allowed to interact for a set amount of time, providing a perspective of the system's dynamic "evolution." Chemical processes in catalytic systems are increasingly being investigated using ab initio molecular dynamics simulations paired with increased sampling approaches. In their rigorous depiction of enthalpic and entropic contributions, these methodologies automatically include finite temperature effects, anharmonicity, and collective dynamics, which can have a major impact on reaction free energy landscapes. This differs from traditional ab initio static methods, which rely on calculating reaction free energies from various coarse-grained representations of the reaction potential energy surface. Ab initio molecular dynamics with enhanced sampling allows for first-principles simulations of systems with increasing complexity, such as solid/liquid catalytic interfaces [1,2].

Description

Computational workflows that integrate Molecular Dynamics (MD) simulations with new data-centric (DC) approaches help speed up the experimental and computational screening and analysis of solvent systems. MD simulations offer atomic locations and velocities of reactant, solvent, and catalyst materials, which can be transformed into data representations and exploited by DC approaches for predictive modelling, feature extraction, and experimental design. Emerging DC approaches such as Convolutional and Graph Neural Networks (CNN/GNN), Topological Data Analysis (TDA), and Active Learning (AL) can use MD and experimental data to predict solvent effects on reaction outcomes for liquid-phase catalytic applications [3].

Another method for investigating atom position in space is molecular dynamics (MD). A dynamic model, in which the nuclear system is put into motion, replaces the single-point model in this approach. The numerical solution of the classical Newtonian dynamic equations is used to simulate the motion. For a given molecule, the collection of potential atom sites yields a conformational ensemble profile. MD can also offer information on the molecules' thermodynamic and kinetic characteristics. The MD can be utilised for protein shape simulations and X-ray structural refining. Molecular dynamics (MD) and related methods are close to becoming routine computational tools for drug discovery. Their primary benefit is that they openly address structural flexibility and entropic consequences. As better algorithms and hardware architectures become more common, this allows for a more precise estimation of the thermodynamics and kinetics associated with drug–target identification and binding [4].

Teaching computational chemistry concepts and tools in undergraduate degree programmes presents significant obstacles. Because of the field's complexity, most courses devote little effort to teaching these technologies and the necessary computer literacy. Furthermore, given the wide range of fields in which computational tools can be employed, it is difficult to provide more than a basic introduction to some of the tools and the physical understanding that they can bring. For instance, training in one area, such as classical molecular dynamics utilising a force field technique, does not guarantee that students will be able to tackle other areas of computational chemistry, such as electronic structure computations. The problem is exacerbated by the fact that many computing tools are outdated [5].

Conclusion

Conformational modifications in nucleic acids are significantly more complicated. In comparison to proteins or complicated RNAs, standard B-DNA has a comparatively simple structure; yet, it is an extraordinarily plastic molecule that undergoes massive conformational changes to adapt to its contact partners. Binding of transcription factors to DNA, for example, is a direct result of the DNA molecule's ability to adapt to the protein surface, as well as DNA sequence recognition.

Conflict of Interest

None.

References

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***Address for Correspondence:** Lobaina Alrhia, Department of Fluid Mechanics, University of Milan, Milan, Italy; E-mail: lobainaalrhia@gmail.com*

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