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REVIEW ARTICLE

Interactive Molecular Dynamics in Virtual Reality for Multidisciplinary Education: Theory and Higher Education Applications

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Abstract This paper explores the integration of virtual reality (VR) technology with molecular simulations to visualize structures, reactions, and behaviors across multiple scientific fields. An emerging tool, Manta, is introduced from its theoretical foundation, along with many immersive and interactive use cases. These virtual cases enable researchers and students to explore the structural properties of materials, to simulate dynamic molecular behaviors, and to observe complex chemical reactions in real time. In case studies of the microscopic mechanisms of aluminum/graphene, organic reactions like the Diels–Alder reaction, and the decomposition processes of energetic materials, Manta illustrates its ability to serve diverse needs. Further, the virtual docking experiment, which provides an ideal scenario for ligand–protein interactions, can be helpful for undergraduate students who are learning computational biology. Regarding computational chemistry, one of the cases describes the structure changes from a quantitative perspective, overcoming the steep learning curve associated with traditional methods. Overall, this paper highlights the potential of VR-enhanced molecular simulations to revolutionize scientific research and education, advancing the fields of molecular dynamics, materials science, and beyond.

Keywords virtual reality, higher education, molecular dynamics, immersive learning

1 Introduction

Atomic-level simulations have begun to play an increasingly important role in higher education, serving both scientific research and education applications (Bennie et al., 2019; Burkholder et al., 2008; Mahian et al., 2019), particularly in the fields of chemistry (Lipkowitz et al., 2000; Popova et al., 2016), materials science (Eremin & Ananikov, 2017; Horike et al., 2009; Lavrentiev et al., 2019), and biology (Gul et al., 2024; Wu et al., 2024a; Yi et al., 2024). Chemistry aims to explain macroscopic phenomena from a microscopic perspective, focusing on the composition, structure, properties, and transformations of matter. Materials science emphasizes the relationship between material properties and their microstructures, while modern biology relies on molecular-level analysis to build an understanding from proteins to observable symptoms. However, intuitive understanding of complex molecular reactions and structures often remains challenging, and current teaching methods in higher education fall short of integrating cutting-edge technology into classroom instruction (Harle & Towns, 2011).

Traditional classroom education primarily relies on two-dimensional (2D) representations, such as text, charts, images, and videos (O'Connor et al., 2018). While effective at conveying information, these methods are limited in helping students understand and explore the dynamics of complex molecular structures. In chemistry and materials science, spatial reasoning skills are crucial for understanding various concepts (e.g., symmetry, crystallography, and stereochemistry) (Carlisle et al., 2015; Stieff et al., 2005). Similarly, in biology, dynamic changes in protein molecules and their secondary/tertiary structures are difficult to represent using 2D methods. Existing 2D tools, such as PyMOL (DeLano, 2002), VMD (Humphrey et al., 1996), VESTA (Momma & Izumi, 2011), and GaussView (Li et al., 2016), allow for some molecular and material structure visualization, but such tools are

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often complex to learn and insufficient for representing the dynamic nature of three-dimensional (3D) structures.

In computational chemistry, interactive molecular dynamics (iMD) in virtual reality (VR) is emerging as a transformative bridge technology to connect the manipulation of molecular structures with practical research and educational demands (Amabilino et al., 2019; Deeks et al., 2020b; Luehr et al., 2015). This technology provides the scientific foundation for VR-enabled modeling, which was recognized as one of the "Top Ten Emerging Technologies in Chemistry 2022" (Gomollón-Bel, 2022). In recent years, the rapid development and increasing accessibility of VR technology have opened new pathways for scientific research and education. Using VR or augmented reality (AR) head-mounted displays (HMDs), users can inspect and interact with molecular models in 3D space, gaining an intuitive experience akin to manipulating physical models (Deeks et al., 2020a; Fung et al., 2019; Seritan et al., 2020). iMD connects molecular dynamics (MD) simulations with 3D visualization engines, allowing users to interact with background simulations in real time and intuitively guide the dynamic evolution of molecular structures (Crossley-Lewis et al., 2023; Deeks et al., 2023; Huang et al., 2010). This technology significantly enhances users' understanding and operational efficiency in a microscopic 3D molecular world, and it serves as an effective alternative to traditional human–computer interactions, such as mouse and screen interfaces.

Although scientific computing, such as density functional theory (DFT) (Orio et al., 2009) and MD (Hargittai, 2023), has achieved significant progress in scientific research, a gap still exists between cutting-edge science and its application in higher education (Hansson et al., 2002; Rom et al., 2013). Breakthroughs in areas such as protein structure analysis (Gul et al., 2024; Wu et al., 2024a; Yi et al., 2024), advanced nanomaterial development (Shah et al., 2024; Torabi et al., 2024; Wu et al., 2024b), and dynamic study of chemical reactions (Zou et al., 2024) remain challenging to integrate into undergraduate courses due to tool complexity and high learning barriers. Moreover, the increasing hardware requirements of technologies like AlphaFold (Jumper et al., 2021) further accentuate this gap, raising an urgent question about how to efficiently incorporate these advancements into higher education.

To address these challenges, our team at Beijing Institute of Technology developed an iMD software program named "Manta" that integrates advanced 3D visualization technology and VR interaction capabilities, enabling the rapid and efficient creation of higher education examples based on cutting-edge science. Manta is highly versatile and applicable to multidisciplinary fields, including mechanics of materials, organic chemistry, materials chemistry, and computational biology. Through the design of diverse teaching applications, Manta aims to bridge the gap between frontier scientific research and classroom education by helping students understand complex molecular structures and reactions intuitively, sparking their interest and creativity and ultimately enhancing the overall teaching experience.

2 An iMD-VR Tool for Multidisciplinary Education: Manta

2.1 | Overview

Manta is designed to combine scientific computing with VR technology, following the "Science + VR" paradigm. Scientific computing provides the physical foundation for regulating the motions of molecules, while VR technology offers interactive design capability and immersive visualization. Manta adopts a modular architecture implementation. Figure 1 illustrates the design overview of the Manta server/client, as well as the application programming interface (API). The VR client is rendered using the Unity3D engine, while the network server coordinates the information flow between the VR client and the physical server (e.g., the MD solver). The API acts as a communication bridge between the VR client and the simulation server; the function of the API is to transmit atomic position data to the physical server and receive the resulting force data. The Manta client then converts this data into real-time simulation visualization while supporting user interaction. The interactive forces applied by users are also fed back to the simulation server, thus creating a closed-loop iMD-VR framework. The underlying MD solver, together with high-quality force fields, supports the scientific foundation of simulated cases. Regarding

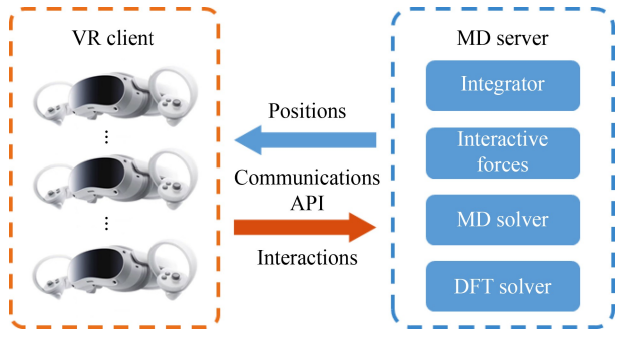

Figure 1 Overview of the Manta server/client design and its application programming interface (API). VR: virtual reality, MD: molecular dynamics, DFT: density functional theory.

case design, Manta does not support structures for which no appropriate force field exists.

For educational uses, Manta is packed as an executable application compatible with the Windows environment, including Windows 10 and Windows 11, while also being compatible with a variety of VR headset devices, such as HTC Vive and PICO 4. This framework supports the scalable integration of VR and MD simulation technologies, leveraging real-time data streaming and interaction feedback for immersive scientific exploration. Manta can also be deployed in remote mode, in which case the physical engine (e.g., the MD server) is set up on high performance cluster and communicates with the local VR client via the internet. Manta deployed on Windows, limited by the local computational power, supports molecular cases with a maximum of 5,000 atoms; in contrast, Manta can handle large-scale molecular cases with up to 80,000 atoms if deployed in remote mode. In both modes, the VR visualization can maintain a real-time frame rate of at least 60 fps. Compared to existing iMD-VR tools, such as Narupa (O'Connor et al., 2018), which supports OpenMM (Eastman et al., 2013), DL_POLY (Todorov et al., 2006), LAMMPS (Plimpton, 1995), DFTB+ (Aradi et al., 2007; Hourahine et al., 2020), and SCINE (Husch et al., 2018), Manta exhibits distinct technical implementations with LAMMPS (Plimpton, 1995) because it supports neural network potentials, specifically deep potential (DP) (Wang et al., 2018; Zhang et al., 2018). This feature significantly enhances both the accuracy and the applicability of material cases, as universal force fields have been rapidly developing in the last five years. For example, the DPA-2 model (Zhang et al., 2024) in the DP framework supports over 73 elements and can drastically reduce computational complexity.

2.2 | Atom Selection and MD Engine

Manta supports iMD based on VR hardware (e.g., a controller) to apply external forces on specific atoms. To provide iMD functionality, Zhao et al. (2022) developed an interactive algorithm that supports the manipulation of atoms, which is consistent with the iMD-VR framework proposed by O'Connor et al. (2019). This algorithm features a range-based selection mode, allowing users to select all atoms within a sphere. Once the atoms are selected, external interaction forces can be applied via controller motions (Figure 2(a)). This approach is particularly useful in the study of chemical reaction pathways between molecules, as it enables researchers to induce chemical reactions by precisely applying interactive forces to molecules.

The force vector $\boldsymbol{F}(t)$ acting on a group of atoms can be expressed in terms of the potential energy V as

$$\boldsymbol{F}(t) = -\frac{\mathrm{d}V}{\mathrm{d}\boldsymbol{q}}, \tag{1}$$

where $\boldsymbol{q}$ is a vector containing the positions of all atoms in the ensemble. The interactive algorithm allows participants to guide MD simulations in real time by dividing V into two components:

$$V = V_{\mathrm{int}} + V_{\mathrm{ext}}, \tag{2}$$

where V_{int} represents the internal potential energy from the force field and V_{ext} refers to the additional potential energy applied by participants. Substituting Equation (2) into Equation (1) yields

$$\boldsymbol{F}(t) = -\frac{\mathrm{d}V_{\mathrm{int}}}{\mathrm{d}\boldsymbol{q}} - \frac{\mathrm{d}V_{\mathrm{ext}}}{\mathrm{d}\boldsymbol{q}}. \tag{3}$$

We use spring potentials because they allow the force to be intuitively enhanced by simply increasing

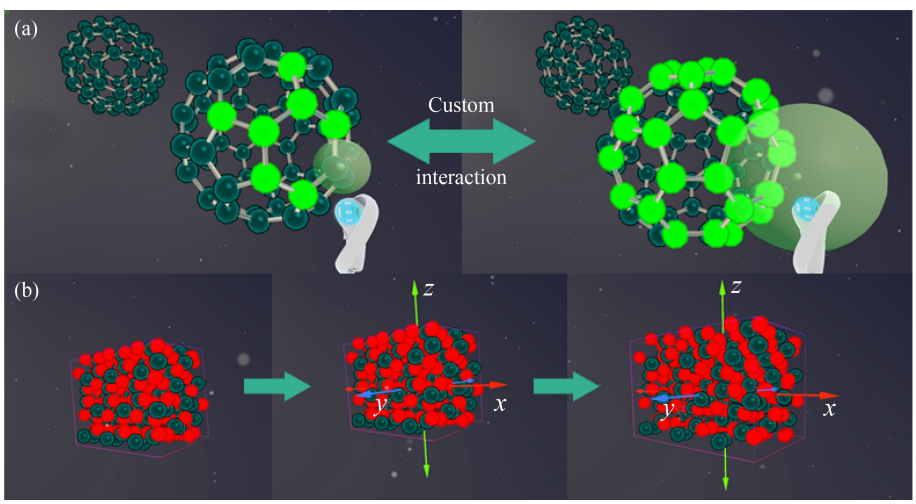

Figure 2 Atom selection and strain adjustment. (a) Custom interaction on the atom selection; (b) strain adjustment along the x-axis on alumina.

the distance per unit time. The expression for the spring potential is

$$\frac{\mathrm{d}V_{\mathrm{ext}}}{\mathrm{d}\boldsymbol{q}} = 2m_j c\left(\boldsymbol{q}_j - \boldsymbol{g}_i\right), \tag{4}$$

where m_j represents the atomic mass of the selected atom j, c is the scaling factor that adjusts the interaction strength, $\boldsymbol{q}_j$ is the position of atom j, and $\boldsymbol{g}_i$ is the interaction position.

During the interaction phase, the controller continuously acts on the selected atom (or group of atoms), allowing participants to dynamically adjust direction and strength by modifying the position of the controller relative to the target atom. To prevent instability in MD integration, the maximum force that may be applied by participants is capped at a predefined threshold. The key to iMD-VR lies in how the interaction parameters in Equation (4) are configured to provide smooth, stable, and intuitive dynamic effects for specific simulation setups without causing excessive disturbances to the system. Manta allows participants to easily modify the scaling parameter c within the VR environment, which can dramatically affect interaction strength during virtual experiments. By integrating MD engines (LAMMPS), Manta relies on LAMMPS-style functionalities to precisely control the thermodynamic conditions of molecular systems (e.g., temperature and pressure). This functional expansion not only enhances Manta's flexibility but also offers additional possibilities for studying complex molecular systems. For example, Figure 2(b) shows the effect of strain adjustment along the x-axis on alumina, further illustrating Manta's powerful capabilities in MD simulations. By combining interactive operations with ensemble controls, Manta presents an efficient, intuitive, and feature-rich microscopic platform for higher education.

2.3 | Molecular Visualization

Manta is a powerful tool in the realm of molecular visualization, as it not only offers interactive functionality but also presents an extensive array of rendering styles. In the domain of scientific visualization, it has comprehensively implemented prevalent models, such as the ball-and-stick model and the van der Waals (VDW) model. The former effectively showcases the connectivity between atoms through a simple yet intuitive representation of spheres (atoms) and rods (bonds), while the latter accurately depicts the spatial extent of atoms based on their VDW radii, providing a more realistic view of molecular shape. To clarify biomolecular structures, especially protein structures, Manta provides a ribbon model (Figure 3), which can vividly highlight the secondary structures within proteins, such as the alpha helices (blue) and beta sheets (red) in Figure 3(a). This enables researchers to quickly identify and analyze the structural features crucial for protein function. To further enrich the user's visual experience and meet diverse research needs, Manta introduces five distinct material rendering options: [Default], known for its ability to enhance the contrast between different atom types; [Bright], which offers a more translucent appearance, allowing for a better view of the internal structure of molecules; [Beautiful], emphasizing the surface texture of molecules to provide a more tactile-like visual perception; [Cartoon], designed to optimize the display of large-scale molecular assemblies; and [Stone], which presents a solid and textured surface to enhance the three-dimensionality and visualization of molecules. By default, carbon, hydrogen, oxygen, and nitrogen atoms are colored green, white, red, and cyan, respectively. However, Manta offers the flexibility to customize the colors of all elements via a color panel, which allows researchers to emphasize specific atoms or functional groups, according to their focus.

Rendering protein molecular surfaces in a VR environment presents a significant challenge. Protein molecules typically contain a large number of atoms, and their molecular surfaces feature irregular pockets and cavities. Consequently, rendering large-scale meshes while maintaining a target frame rate of 60 fps is quite challenging. To address this, Manta provides a visualization mode in which the physical engine is disabled. Instead, it uses a custom API based on a surface interpreter (i.e., the MSMS program) (Sanner et al., 1996) to render the solvent excluded surface of proteins. Next, physical constraints are assigned to the generated surface mesh by computing the molecular forces between protein and ligand. After applying the Lennard-Jones parameters from the GROMACS force field (Bjelkmar et al., 2010), Manta uses an adjustable cutoff distance to dynamically filter valid atom pairs between the protein and ligand to estimate the forces on small molecules. This implementation prevents surface penetration during virtual docking experiments. Figure 3(b) displays the molecular surface of the DNA polymerase in the Monkeypox virus and cidofovir diphosphate (Protein Data Bank Identifier (PDBID): 8J8G) with an opacity of 1 (left panel), as well as the molecular surface of adaptor protein Grb14 (PDBID: 2AUG) with an opacity of 0.7 (right panel).

In addition to rendering molecular positions and structures, Manta supports specialized visualization methods, such as atomic trajectories, kinetic energy, and force visualizations (Figure 3(c)). The atomic trajectory visualization illustrates the motion paths of atoms, aiding users in analyzing dynamic behaviors, and the kinetic energy visualization renders the atomic color according to the corresponding kinetic energy, supporting the study of energy distribution and dynamic properties. Finally, the force visualization

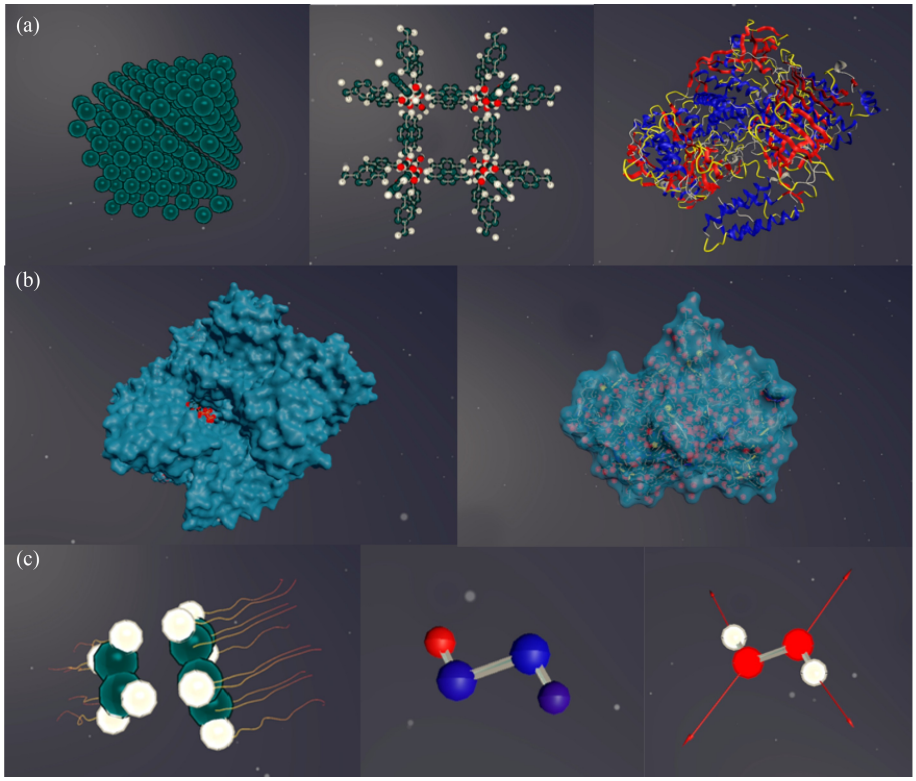

Figure 3 Molecular visualization in Manta. (a) Molecular model (from left to right): van der Waals, ball-and-stick, and ribbon model; (b) molecular surfaces with different transparencies; (c) visualization method (from left to right): trail, kinetic energy, and force visualization.

intuitively represents the distribution of interatomic forces, which is useful when examining detailed interactions between atoms.

2.4 | Interactive Molecular Design

Manta allows users to freely add or remove atoms and molecules within a molecular case study. This flexible and interactive design not only meets users' personalized needs for molecular systems but also greatly facilitates molecular editing and structure optimization. When users add or remove atoms, the client instantly modifies the molecular structure by inserting atoms at precise coordinates or deleting the selected atoms from the atom list. Next, the updated atomic position data are transmitted to the MD server via API interfaces. This functionality only works with reactive force fields, such as ReaxFF models (van Duin et al., 2001), as Manta does not require complex manipulation of molecular topology when adding or deleting atoms. Figure 4(a) illustrates the process of adding oxygen atoms (red) and removing hydrogen atoms (white). To further enhance the molecular design process, a variety of common atomic groups are preloaded (e.g., $-CH_3$, –OH, and $-NH_2$), and users can quickly assemble these for different design purposes.

The use of periodic boundary conditions (PBCs) is common in molecular simulations, and the technique plays a crucial role in molecular design. By simulating the boundary effects of an infinite system, PBCs effectively reduce boundary effects while conserving computational resources. In Manta, PBC functionality is implemented to allow duplication along three axes. Figure 4(b) demonstrates the duplication results of an alumina structure under PBCs. With this feature, users can intuitively observe the periodic characteristics and overall structure of the material, which is particularly useful for crystal structures.

3 Manta Applications: Multidisciplinary Education

After the initial release of Manta in 2020, a pioneering demonstration was made in the course Combustion Basics at Beijing Institute of Technology (Zhao et al., 2022). Since then, several additional examples have been designed and applied in multiple disciplines, including chemistry, mechanics, and biology, at various universities.

3.1 | Mechanics of Materials

Mechanics of materials is a discipline that studies the

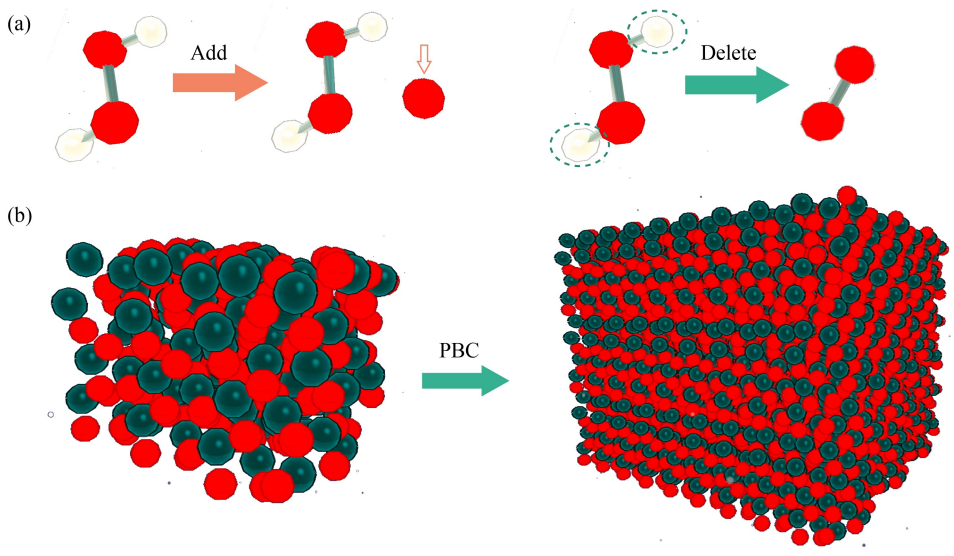

Figure 4 Molecular design in Manta. (a) Operation of adding and deleting atoms; (b) operation of periodic duplication. PBC: periodic boundary condition.

strain, stress, strength, stiffness, stability, and failure limits of different materials under various external forces; the structure of a material directly determines its physical properties and performance. Therefore, understanding microstructure is crucial for revealing the origins of material strength, elasticity, and plasticity, thus clarifying and simplifying the design of new materials. Based on this, a series of molecular examples were created to explore the specific structures in depth. These examples can help researchers visually analyze structural features and simulate dynamic behavior under varying conditions while providing important references for material design and optimization.

Figure 5 shows the molecular structures of representative materials in Manta. All these cases have been used in the virtual experiment of mechanics of materials lectured by Professor Jing Xie at Beijing Institute of Technology since 2022. All cases were performed under the NVT ensemble at a constant temperature of 300 K, with PBCs applied. In the case of aluminum and aluminum oxide, the ReaxFF model was employed incorporating Al–O interactions (Muraleedharan et al., 2020). Other cases include the ReaxFF model developed by Hou et al. (2022) for C/H/O/N/S/P elements.

Aluminum (Al): Aluminum (Figure 5(a)) has a face-centered cubic crystal structure, with atoms

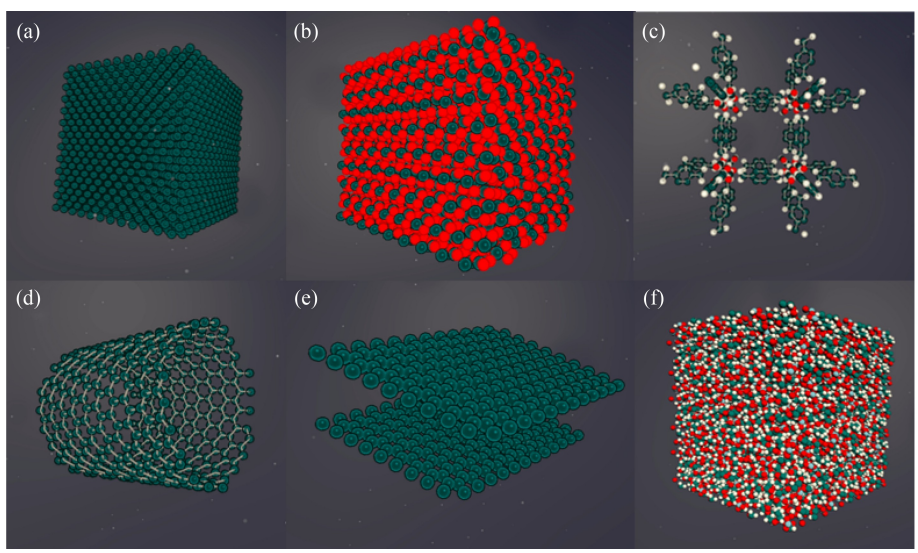

Figure 5 Examples in mechanics of materials using representative molecular structures. (a) Aluminum; (b) aluminum oxide; (c) metal-organic frameworks; (d) carbon nanotubes; (e) graphene; (f) nitrate ester plasticized polyether matrix. The number of atoms in the examples are 256, 270, 616, 456, 432, and 608, respectively.

densely packed to form a highly symmetrical organization. This structure gives aluminum excellent electrical conductivity, thermal conductivity, and ductility. By observing its microstructure in Manta, students can intuitively understand its high conductivity and good plasticity, which are key for designing and optimizing aluminum alloys. The unique characteristics of aluminum have led to its wide use in aerospace, automotive industries, and other fields, especially in applications requiring lightweight and high-strength materials.

Aluminum oxide (Al_2O_3): The microstructure (Figure 5(b)) and mechanical properties of aluminum oxideare primarily determined by its crystal structure and bonding characteristics. α-Al_2O_3 adopts a hexagonal close-packed structure, and its strong covalent–ionic bonds endow it with high hardness and compressive strength. The tightly packed structure of Al_2O_3 enables it to exhibit excellent stability under high-temperature and high-pressure conditions.

Metal-organic frameworks (MOFs): The mechanical properties of MOFs are primarily determined by their structures (Figure 5(c)), which consist of metal ions or clusters connected to organic ligands through coordination bonds. The pore structure and surface characteristics of MOFs help them withstand the mechanical forces generated by gas pressure during high-pressure gas storage and separation processes, and the potential of MOFs regarding gas adsorption, separation, and catalysis can be derived. The mechanical properties of MOFs directly impact their durability and performance in practical applications, making the study of their mechanical behavior crucial for optimizing performance.

Carbon nanotubes (CNTs): The mechanical properties of CNTs are primarily determined by their unique tubular structure (Figure 5(d)) and arrangement of carbon atoms. CNTs are formed by rolling a single layer of graphene into a tube that exhibits an extremely high aspect ratio and exceptional mechanical properties. The carbon–carbon bonds in CNTs give them extremely high tensile strength and elastic modulus, making them one of the strongest lightweight materials. Exploring the microstructure in Manta allows for the widespread applications of CNTs in composite materials, nanomechanical systems, and sensors to be fully appreciated.

Graphene: The mechanical properties of graphene stem from its 2D honeycomb-like structure of carbon atoms (Figure 5(e)). From a mechanical perspective, graphene exhibits extremely high in-plane stiffness and strength, along with excellent flexibility and elasticity. These unique mechanical properties make it widely applicable in flexible electronic devices, composite materials, and high-strength films. The combination of unique electronic structure and adaptable mechanical properties provide theoretical support for its applications in cutting-edge technologies, such as supercapacitors, batteries, and sensors.

Nitrate ester plasticized polyether (NEPE) propellant: The microstructure (Figure 5(f)) and mechanical properties of NEPE propellant depend on crosslinking density and molecular arrangement. The NEPE curing process centers on reactions between the hydroxyl groups (–OH) of polyether polyols (e.g., PEG-400) and the isocyanate groups (–NCO) of curing agents (e.g., N-100 or HDI). These groups form urethane bonds (–NH–CO–O–), creating a 3D crosslinked network. Using Manta, one can identify the microstructure of the crosslinking network in the NEPE matrix.

3.2 | Materials Chemistry

In materials chemistry, understanding the chemical properties of materials is key to advancing their applications. Here, we present two virtual experiments prepared in Manta to illustrate the structures of energetic materials and their decomposition behavior under high-temperature conditions. Both cases were used in an organic chemistry course instructed by Professor Zhiyue Han at Beijing Institute of Technology. The force fields for all simulations were taken from Cao et al. (2022).

In the first case, an example library containing nine common explosive molecules was constructed (Figure 6). This library contains 209 atoms and aims to assist students in learning these molecular structures. Simulations were performed under the NVT ensemble at a constant temperature of 300 K. By observing the key structural features of these molecules, students can reconstruct the 3D structures instead of the 2D projection shown in textbooks. For example, the CL-20 molecule, which is one of the most powerful explosives ever discovered, exhibits a complex cage structure featuring symmetry in specific directions. Typically, students struggle to conceptualize the cage, but Manta mitigates this education bottleneck by providing an immersive visualization of the molecular structure. Further teaching points include the identification of weak bonds in the molecular structure, which can be accomplished by turning on the highlighting of molecular forces. By integrating the molecular structures in Manta with the content in textbooks, students achieve a much better learning outcome and gain a deeper understanding of the molecular structures of energetic materials.

Energetic materials release their inherent high-density energy via complex thermal decomposition. As the temperature increases, explosive molecules typically undergo a series of complex decomposition stages, including bond cleavage and the formation of

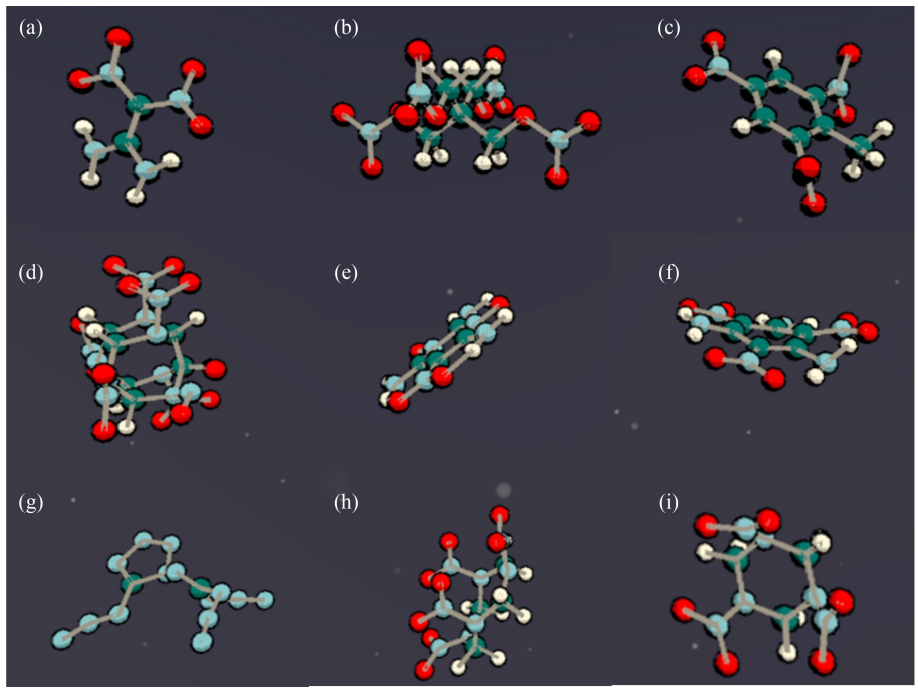

Figure 6 Nine explosive molecules in Manta. (a) FOX-7; (b) PETN; (c) TNT; (d) CL-20; (e) ICM-102 (Chu et al., 2022); (f) TATB; (g) C_2N_{14}; (h) HMX; (i) RDX. Green, white, cyan, and red represent carbon, hydrogen, nitrogen, and oxygen atoms, respectively.

intermediates, ultimately releasing large amounts of heat and gas. Understanding this process is crucial for practical applications of materials; however, most students, hindered by the complexity of such reactions and the classical teaching methods in higher education, cannot comprehend the detailed evolution image. To resolve this issue, a set of virtual cases was created in Manta. In the second experiment, two typical explosive molecules, CL-20 and TNT, were selected from the example library to construct a case of 57 atoms. The molecules' decomposition processes were demonstrated under NVT ensemble conditions at a constant temperature of 2000 K, with PBCs. In Manta, MD simulations can be used to illustrate the dynamic changes of molecules in a high-temperature environment, as well as the reaction pathways and state transitions, and students may tune the temperature setting to monitor the impact of temperature on decomposition. As seen in Figure 7, the decomposition rate of CL-20 was higher than that of TNT. The first decomposition product in the CL-20 case was NO_2 in the second snapshot, while a hydrogen radical is being released from the TNT decomposition in the third snapshot. This was mainly due to the low activation energy in the N–NO_2 scission of CL-20 decomposition. The subsequent reactions involved the formation of H radicals, CH_2N, NO_2, and HCN. In contrast, the decomposition process of TNT was relatively slow, releasing H radicals, NO_2, and CO. From these observations, students can build a better understanding of decomposition at high temperatures.

3.3 | Organic Chemistry

Organic chemistry primarily focuses on the structures, reactions, and synthesis methods of organic compounds, as well as the dynamic behavior of molecules over time. It involves intra-molecular conformational rearrangements of molecules and inter-molecular reaction mechanisms, such as nucleophilic substitution (SN2) and elimination (E2). In-depth discussion of these reactions provides important theoretical foundations and experimental guidance for organic synthesis. In a previous higher education application, our team collaborated with Professor Yongxin Tang at Nanjing University of Science and Technology to design a set of virtual experiments for organic chemistry using Manta (Liu et al., 2024). Here, we briefly review three representative virtual experiments in organic chemistry. The force fields for all simulations were taken from Zhang et al. (2009). The temperature was maintained at 300 K in the NVT ensemble, and PBCs were applied.

3.3.1 Central C–C Bond Rotation of n-Butane

This virtual experiment demonstrates the free rotation of single bonds within a molecule and the resulting conformational changes, providing an intuitive example of dihedral motions in molecules. In this case, users can rotate the central C–C bond in *n*-butane, observing the transition between different conformations, by using a

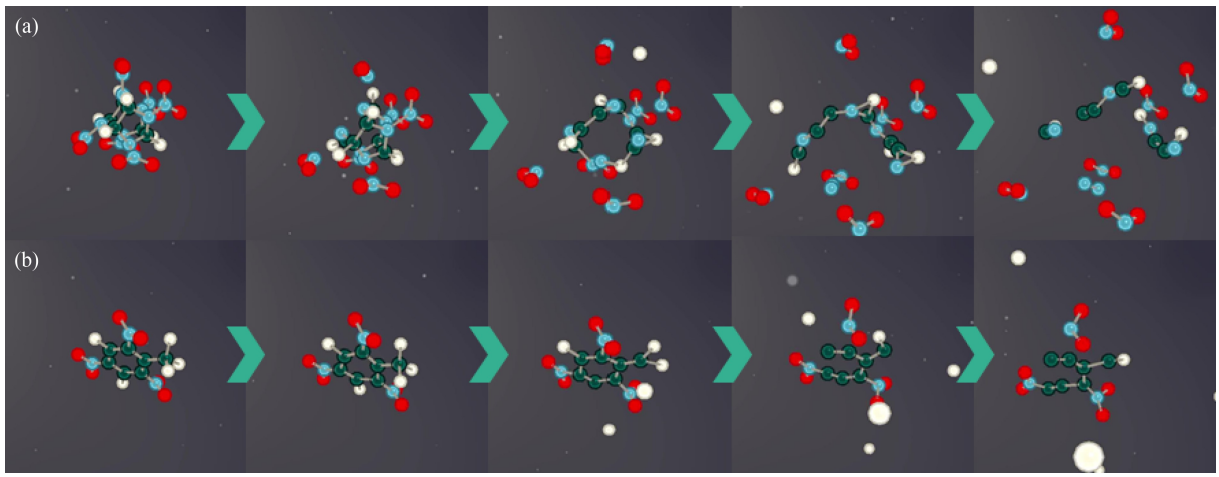

Figure 7 Decomposition reactions of (a) CL-20 and (b) TNT at 2000 K in Manta.

handle to drag the carbon atoms. Figure 8(a) illustrates the conformational change of the C–C bond rotation on textbooks; Figure 8(b) shows the corresponding state changes computed using the DFT method by Gaussian 16 software; and Figure 8(c) depicts the interactive operations in Manta, which allow users to observe the changes in molecular conformations at each rotation step. This interactive process clarifies how single-bond rotation influences molecular structure.

3.3.2 Diels–Alder Reaction of 1,3-Butadiene with Ethene to Form Cyclohexene

This classic [4 + 2] cycloaddition reaction showcases the formation of double- and single-bond, which are important synthetic reactions in organic chemistry. In the virtual experiment, users manipulate the angles and positions of reactants to observe how 1,3-butadiene and ethene react to form cyclohexene. Figure 9(a) is a textbook illustration of the reaction pathway. Figure 9(b) demonstrates the corresponding state changes computed using the DFT method by Gaussian 16 software. Figure 9(c) illustrates the interactive operations in Manta that enable users to actively engage in the reaction and visually understand the formation of reaction intermediates. This feature provides valuable insight into the mechanisms of cycloaddition reactions and bond formation.

3.3.3 Electrocyclic Ring Opening of Cyclobutene

This reaction investigates the ring-opening process of molecules under thermal or photochemical conditions. In the virtual experiment, users observe the ring-opening process of cyclobutene under various conditions, focusing on hydrogen bond flipping and changes in the C–C bond distances. The experiment requires users to modify the temperature and observe the molecule transitions from a ring structure to an open form via bond scission (Figure 10). This simulation provides an in-depth understanding of the dynamics of electrocyclic reactions and the influence of external conditions on molecular structure.

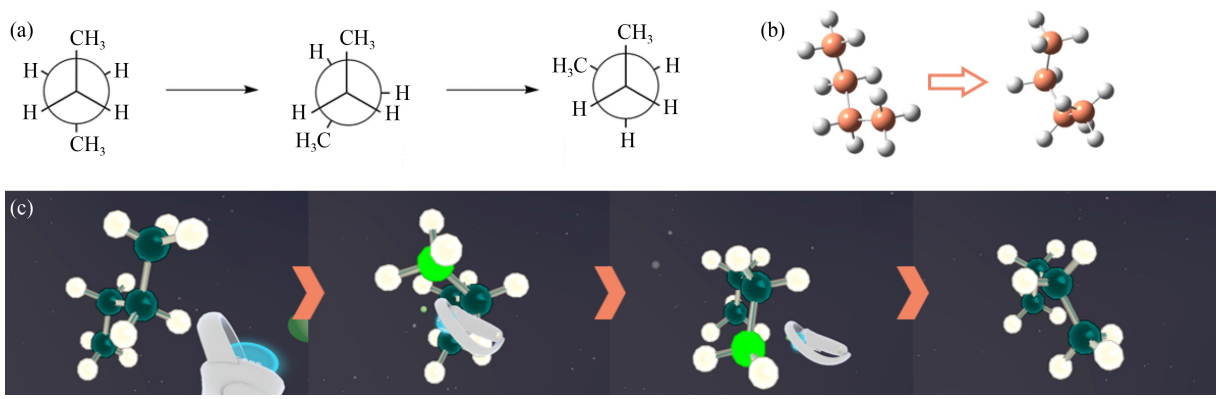

Figure 8 Central C–C bond rotation of *n*-butane. (a) Drawing on textbooks; (b) geometry animation computed by Gaussian 16 software; (c) interactive operations in Manta.

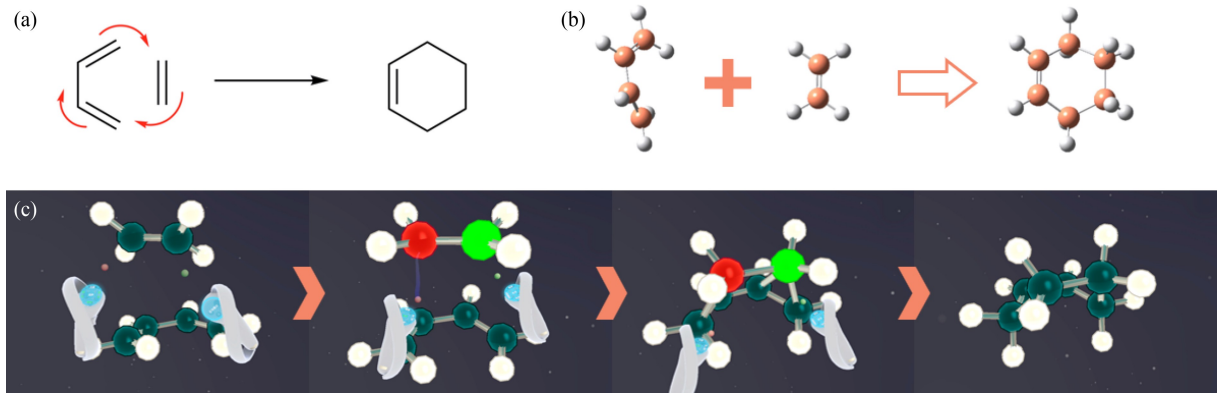

Figure 9 Diels–Alder reaction of 1,3-butadiene with ethene to form cyclohexene. (a) Drawing on textbooks; (b) geometry animation computed by Gaussian 16 software; (c) interactive operations in Manta.

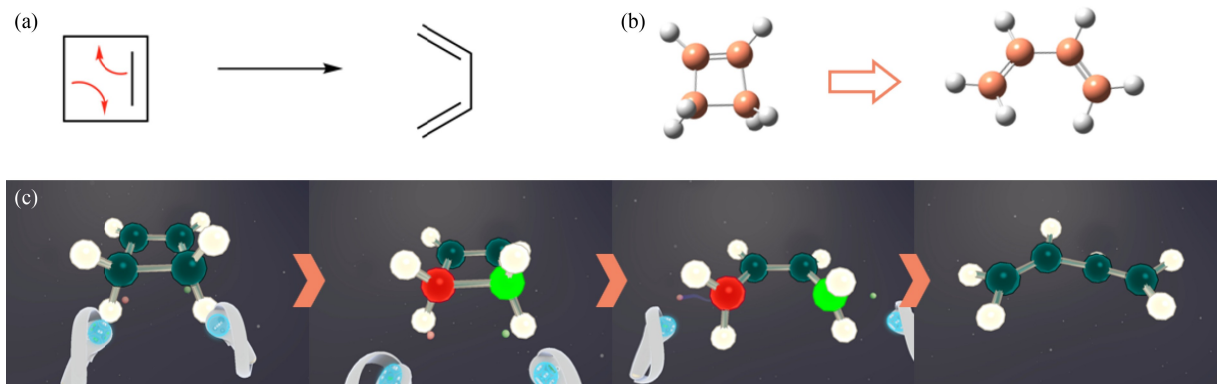

Figure 10 Electrocyclic ring opening of cyclobutene. (a) Drawing on textbooks; (b) geometry animation computed by Gaussian 16 software; (c) interactive operations in Manta.

3.4 | Computational Biology

Computational biology is an interdisciplinary field that integrates computational chemistry and biology, leveraging computational simulations to study the functions of biological systems. This requires scientists to extract valuable information from vast biological datasets. However, the field lacks powerful tools for learning, particularly regarding understanding complex biological structures and their dynamic behaviors, which are crucial to the teaching process. In the context of drug design education, it is essential to master the characteristics of target structures and delve into the interaction mechanisms between small-molecule drugs and their targets.

To meet these teaching needs, Manta features efficient rendering of large-scale molecules, ensuring a smooth operational experience when displaying complex biological structures. The spatial configurations of proteins can be clearly visualized in Manta to help students intuitively understand their 3D characteristics. Figure 11(a) displays Manta's atomic configuration of the DNA polymerase in the Monkeypox virus and cidofovir diphosphate (PDBID: 8J8G). The left panel of Figure 11(a) illustrates the ribbon representation of the secondary structure. The blue, red, and yellow regions represent α-helices, β-sheets, and unstructured sequences, respectively. The right panel presents the full atomic visualization for comparison. Figure 11(b) showcases the double-helix structure of a DNA fragment (1904 atoms), visualizing the base-pair interactions. Figure 11(c) presents the molecular structure of the five nucleotide bases within DNA. This detailed display allows for an in-depth exploration of the molecular foundation underlying genetic information encoding, providing viewers with a comprehensive understanding of the fundamental structures that carry the genetic blueprints of life. Beyond visualization of molecular structures, Manta employs advanced surface rendering technology to highlight the details of molecular surfaces, such as binding sites, which are critical for drug design. Furthermore, Manta integrates efficient human–computer interaction algorithms, allowing users to perform real-time operations and exploration in a virtual environment. For instance, students can use Manta to conduct virtual molecular docking experiments, observe how small-molecule drugs bind to

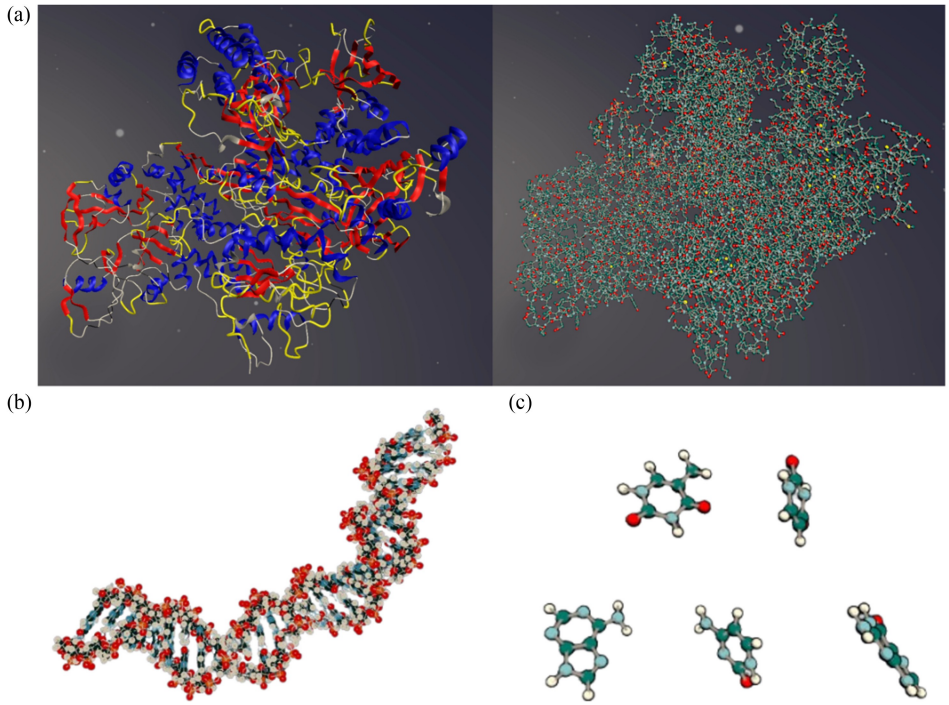

Figure 11 Molecular examples of proteins and DNA. (a) DNA polymerase in the Monkeypox virus and cidofovir diphosphate (PDBID: 8J8G); (b) DNA double-helix structure (1904 atoms); (c) DNA base pairs.

their targets, and analyze the underlying interaction mechanisms.

Molecular docking is a critical technique in drug design, but no currently available tool can effectively render the complex 3D binding structures. By simulating the binding modes and interaction strengths between small-molecule drugs and biological macromolecules (such as proteins and nucleic acids), Manta provides essential theoretical support for the design of drug molecules. To ease teaching of molecular docking, a virtual example mimics the interactions between the DNA polymerase in the Monkeypox virus and cidofovir diphosphate. Figure 12(a) highlights the specific binding site between the DNA polymerase in the Monkeypox virus and cidofovir diphosphate; Figure 12(b) presents the molecular structure of cidofovir diphosphate; and Figure 12(c) shows the virtual docking experiment created in Manta. In this case, users can observe and manipulate how cidofovir diphosphate binds to DNA polymerase through

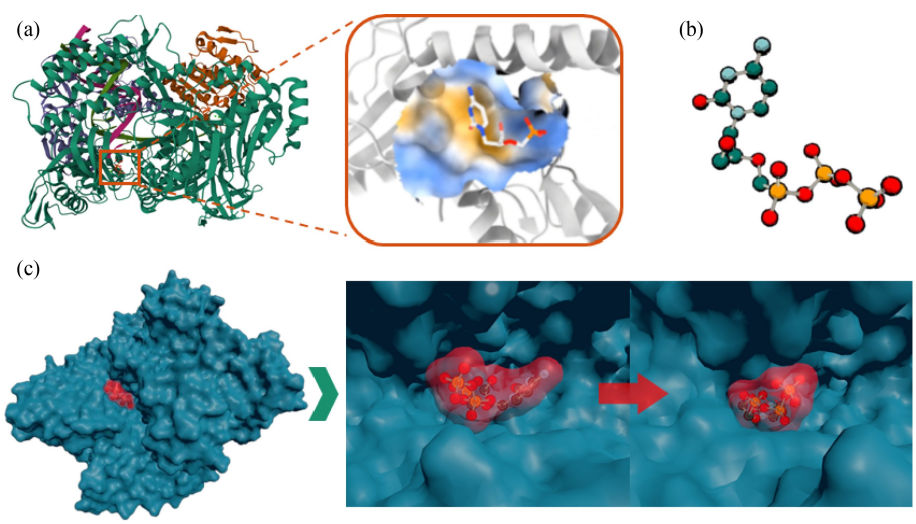

Figure 12 Examples of ligand binding to a protein in Manta. (a) Schematic of cidofovir diphosphate binding to DNA polymerase in the Monkeypox virus; (b) molecular structure of cidofovir diphosphate; (c) examples of cidofovir diphosphate binding to DNA polymerase in Manta.

human–machine interactions, providing a real-time exploration of intermolecular interactions. At the 2024 Global MOOC and Online Education Conference, the above virtual docking experiment was presented as an AI-enabled higher education application scenario.

During the experiment, users observe the molecular surface structure of DNA polymerase in a virtual space, independently exploring and locating suitable binding sites. With the help of VR handles, users can precisely manipulate cidofovir diphosphate molecules and perform real-time docking with DNA polymerase. The system dynamically provides feedback on the collision effects during the docking process, helping users perceive the intermolecular interaction forces and optimize the docking process. Ultimately, users achieve precise docking by traversing through spatial obstructions and adjusting the docking angle of cidofovir diphosphate to reach the optimal binding state. This virtual docking experiment, through immersive experience and real-time interaction, enables students to mimic microscopic docking as if playing a video game, through which they gain deeper insight into the mechanisms of intermolecular interactions. At the same time, the experiment effectively enhances students' practical skills, spatial thinking abilities, and interest in scientific exploration. In addition, by integrating computational biology modeling and simulation techniques, molecular docking can efficiently screen the small-molecule compounds that bind to specific docking sites. This approach establishes a solid theoretical foundation for drug development and provides a potentially valuable tool in drug research.

3.5 | Computational Chemistry

Computational chemistry focuses on the energy distribution and dynamic behavior of molecular systems, with its core objective being a quantitative view of reaction calculations and simulations. The potential energy surface (PES), as a key tool for describing the energy evolution of molecular systems, is indispensable in reaction mechanism research. However, existing tools face significant challenges in efficiently sampling PES and visualizing complex reaction processes, and the necessary scientific software requires a high level of theoretical background that is too advanced for many undergraduate students. To address this issue, Manta, through its human-friendly interface and immersive visualization capabilities, enables students to easily participate in real-time iMD simulations, observe the synergistic process evolutions, and thereby establish an intuition for the intrinsic relationship between structure and energy. This immersive experience significantly lowers the learning barrier and transforms abstract chemical dynamics concepts into vivid and dynamic visual processes, effectively addressing the limitations of traditional teaching tools.

For example, Manta provides an innovative teaching scenario for studying chemical bond dynamics in the bond-breaking experiment (Figure 13(a)), in which users manipulate two CH_3 groups to break the C–C bond while the system simultaneously displays the molecular configuration evolution. The potential energy decreases from −786 kcal/mol (1 kcal/mol = 4.184 kJ/mol) through −723 kcal/mol to a final −695 kcal/mol. In the case of bond rotation (Figure 13(b)), the rotation of the CH_3 group in ethane causes a harmonic-like energy evolution. Through real-time operational feedback and 3D dynamic visualization, these experiments transform abstract chemical bond behaviors into tangible physical parameter changes, effectively building a cognitive bridge between structure and energy.

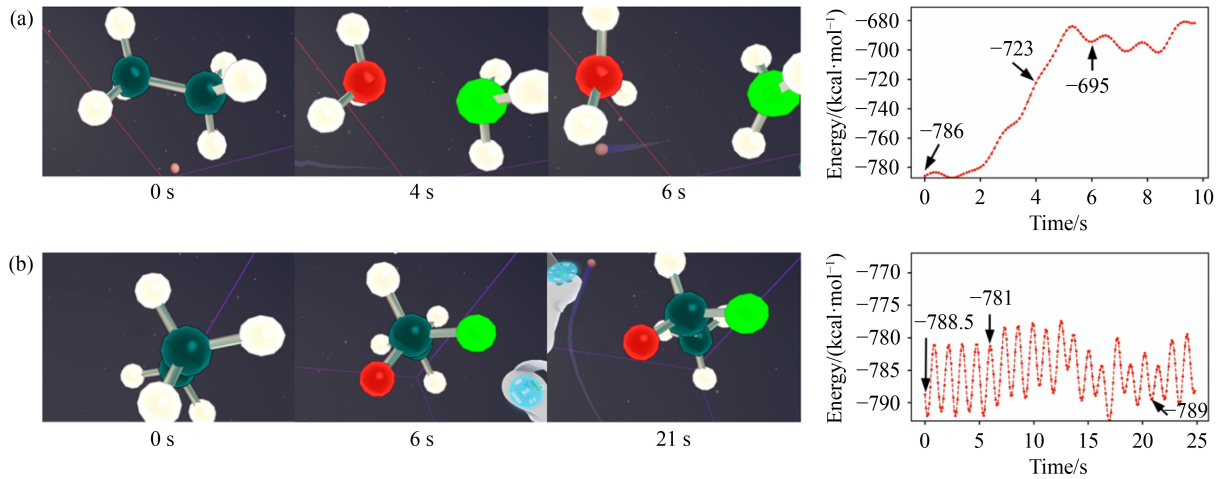

Figure 13 Sampling energy changes via configuration operation using handlers in Manta. (a) Bond scission; (b) bond rotation experiment. The left panels illustrate the dynamic changes during bond scission/rotation, while the right side shows the corresponding energy changes.

4 Instructional Application

On April 22, 2025, Professor Song Chen from Peking University adopted Manta in a graduate course entitled "Molecular Dynamics." The session included a virtual docking experiment involving the DNA polymerase in the Monkeypox virus and cidofovir diphosphate (PDBID: 8J8G). Nine students from different majors, such as biochemistry, physical chemistry, bioinformatics, and biophysics, were presented with the in-class teaching exercise. The course employed a three-phase instructional design (Figure 14), i.e., theory explanation, case demonstration, and group exercise. It began with a background and introduction, which included biological characteristics, molecular docking, and the VR-enabled modeling approach (i.e., Manta). This was followed by a live demonstration of the core steps, such as structural visualization, molecular surface modeling, ligand generation, and docking site screening. During the group practice phase, the students were divided into three teams to conduct virtual docking experiments. The effectiveness of the instruction was evaluated through a quantitative questionnaire, the key feedback results of which are summarized in Figure 15. These questions aimed to assess whether Manta could provide students with an enhanced learning experience. Nine representative questions were selected (from a total of 16) for inclusion in this paper. The questionnaire used a 5-point Likert scale (1 for "strong disagreement", 5 for "strong agreement").

In the evaluation of software adaptability (Q1–Q2), the tool performed well in both disciplinary relevance and situational authenticity, achieving nearly perfect scores. In particular, the students praised Manta's restoration of protein structures and simulation of drug interaction processes, confirming that the tool effectively supports the core requirements of the teaching exercise in computational biology. Regarding software usability (Q3–Q5), Manta demonstrated significant advantages, with all three metrics averaging above 4. Nearly 67% of participants explicitly acknowledged the intuitiveness of its operational workflow, and most of the students claimed that they could master basic operations within 10 minutes. Students' feedback on interaction design in Manta was mixed, as 67% of the surveyed students reported outstanding performance in task interactivity and multimodal feedback (e.g., the immersive 3D visualization capability and realistic haptic feedback during molecular collisions), but the remaining 33% noted that the weight and style of current VR headsets caused noticeable physical discomfort, and prolonged usage led to symptoms of visual motion sickness. This negative feedback indicates the need for further optimization of human–computer interaction design in VR equipment.

In terms of teaching effectiveness (Q6–Q9), the dynamic interactive design showcased unique strengths. By allowing real-time adjustments to the relative positions of drug molecules and receptor proteins through applied forces, students could intuitively

Figure 14 Instructional application scene of Manta in computational biology. (a) Theory explanation; (b) a case demonstration performed by the teacher; (c) an exercise guided from a student tutor; (d) student group exercise.

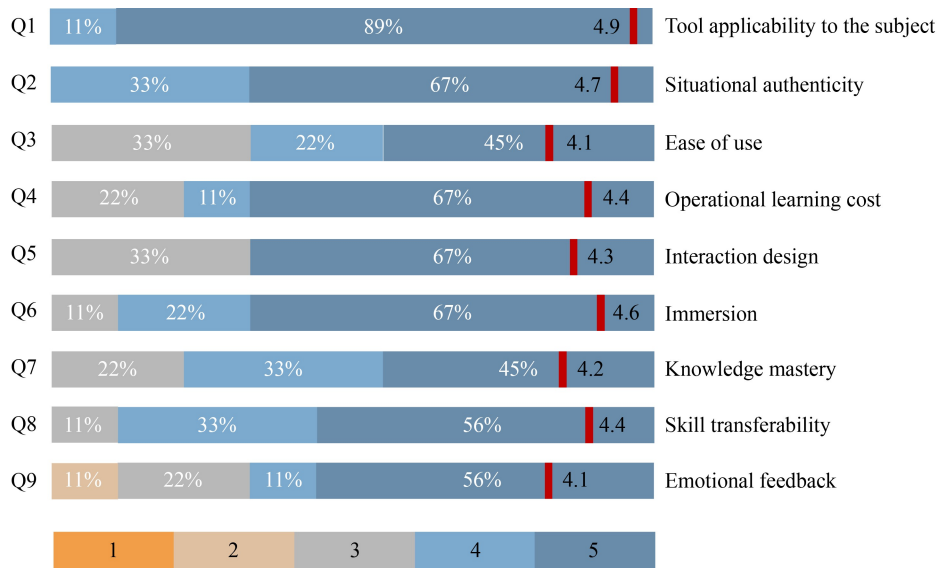

Figure 15 Distribution of the students' preferences for the applications of Manta in the class experiments. The mean values are represented by solid lines.

perceive ligand–receptor interactions. The participants agreed that Manta's "drag-and-explore" feature noticeably simplified the discovery of potential binding sites. In addition, while demonstrating significantly improved classroom engagement, the students exhibited enhanced learning interest and reduced anxiety levels, and most importantly, acquired skills that are directly transferable to authentic research applications. These outcomes further validate the importance of virtual simulation technology in classroom teaching.

5 Conclusions and Future Perspective

In this work, we comprehensively demonstrate the immense potential of the "Science + VR" concept across multiple scientific fields, including mechanics of materials, organic chemistry, materials chemistry, computational biology, and computational chemistry. Utilizing tools such as Manta, we can create highly interactive simulation environments that enable the visualization of molecular structures, the animation of chemical reactions, and engagement in hands-on experiments. This technology not only enhances the learning experience for students and researchers but also provides critical theoretical support and practical guidance for new material design, reaction pathway optimization, and drug development. The concept of "Science + VR," through the deep integration of scientific computing methods (e.g., MD) and VR technology, offers novel possibilities for scientific research and education, addressing the limitations of traditional tools in micro-scale research. Built from a multiscale design philosophy, Manta reflects the world through a set of colorful lenses, aligning complex patterns within the chaos and sparking enlightenment across intertwined fields.

The integration of VR technology with MD simulations, as demonstrated by Manta, is bringing profound transformations to scientific research and education. In the future, Manta will further enhance its capability to handle large-scale and complex molecular systems, particularly in fields such as computational biology and nanomaterials. This will provide researchers with unprecedented levels of detail, aiding in the exploration of complex biological processes and material behaviors. Through real-time data acquisition and dynamic adjustment of simulation parameters, Manta will create a more interactive and immersive research environment, improving the intuitiveness and flexibility of molecular system exploration. Moreover, the ongoing integration of AI will significantly enhance automated molecular design, prediction of material properties, and optimization of molecular configurations. In the field of drug discovery, AI can simulate interactions between drugs and target proteins, and identify potential drug candidates to accelerate the drug development process.

In the field of education, Manta has the potential to provide students with personalized learning experiences. By analyzing students' interaction data, Manta can tailor content to individual learning needs, helping students better understand complex molecular science concepts. Furthermore, Manta can organize disciplines (e.g., chemistry, biology, physics, and materials science), offering a cross-disciplinary learning

platform, and the virtual experiments help students understand both microscopic behaviors and real-world applications.

In the future, Manta will support multi-user environments, fostering global scientific collaboration. Researchers and students from different regions will be able to conduct real-time experiments and share data within the same virtual space to accelerate scientific discovery. Manta will also evolve into a comprehensive virtual chemistry laboratory, supporting functions such as virtual chemical reactions and spectral analysis and providing a low-cost and safe experimental platform that is particularly suitable for scenarios in which the traditional experiments are high-risk or costly. With advancements in hardware, Manta will leverage new technologies, such as haptic feedback, hand-tracking, and eye-tracking, to further enhance immersion and interaction. Additionally, the integration of cloud computing resources will support large-scale simulations, improving accessibility and computational efficiency. The education cases in Manta will also be expanded into emerging fields, such as drug discovery, energy materials, and catalysis, driving the optimization of new materials. As technology continues to advance, Manta will play an increasingly important role in scientific research, education, and cross-disciplinary collaboration, facilitating and catalyzing global innovation.

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Authors Contributions Jinyu Ma drafted this study and made substantive contributions to the methodology and software. Huawei Cao participated in data curation and investigation. Ding Nie contributed to data curation and formal analysis. Dongping Chen was responsible for conceptualization and project administration. All authors reviewed and approved the final published version of the study, ensuring the accuracy and scientific integrity of the research content.

Conflict of Interest The authors declare that they have no conflict of interest.

Ethics Statements The authors declare that their Institutional Ethics Committee confirmed that no ethical review was required for this study. Written informed consent for participation was not required because all participants' data was anonymized before the statistical analyses were done.

Data Availability Statements The authors confirm that all data generated or analysed during this study are included in this published article.

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