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Analysis of Teaching Reform Strategies for the Molecular Dynamics Course in Universities

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Abstract: As a core discipline connecting the motion of micro-particles with the properties of macro-substances, molecular dynamics is an important professional course for majors such as physics, chemistry, and materials science in universities. With the intensification of interdisciplinary integration and the rapid iteration of cutting-edge technologies, the traditional teaching model of molecular dynamics can no longer meet the demand for cultivating innovative and practical talents. Based on this, this paper conducts research on the teaching reform strategies for the molecular dynamics course in universities, systematically analyzes the problems existing in the traditional teaching of the course, clarifies the core value of teaching reform, and proposes targeted teaching reform strategies. The aim is to improve the quality of course teaching, help students consolidate theoretical foundations, enhance practical and innovative abilities, so as to adapt to disciplinary development and industry needs.

Keywords: Universities; Molecular dynamics; Teaching reform; Teaching evaluation

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1. Introduction

Based on the principles of classical mechanics, molecular dynamics reveals the inherent connection between the macro-properties of substances and micro-motion laws through computer simulation of the motion behavior of micro-particles. It is widely used in cutting-edge fields such as materials design, drug research, and development. As a core course connecting basic theories with scientific research practice for majors like physics and materials science in universities, it undertakes the important mission of cultivating students' micro-cognition, quantitative analysis, and computer simulation practical abilities [1]. With the development of computer technology, molecular dynamics simulation software and algorithms are continuously upgraded, and the research system and scale are constantly expanding. However, most universities still adopt the traditional teaching model, which is difficult to adapt to disciplinary development and industry needs. Therefore, exploring teaching reform strategies for the molecular dynamics course in universities is of great practical significance.

2. Problems existing in the traditional teaching of the molecular dynamics course in universities

2.1. Outdated teaching content

The traditional teaching model mostly focuses on imparting classical theories and basic algorithms, but the textbook update is lagging behind, making it difficult to reflect the latest disciplinary developments in a timely manner. On one hand, it overemphasizes the thorough teaching of basic knowledge, lacking consideration of new technologies such as machine learning-assisted molecular dynamics and multi-scale simulation, as well as cases of constructing complex systems such as biological membranes and polymer composites; on the other hand, software skill training is only limited to the simple application of common software such as GROMACS and LAMMPS, without teaching the use of their latest functional modules, and there is a lack of courses on custom potential function setting and data analysis skills. This leads to students having an outdated knowledge structure, resulting in a disconnect between scientific research practice requirements and industry development trends.

2.2. Weak practical teaching

Practical teaching is a key path for the organic integration of theoretical knowledge and application skills, and its importance is self-evident. Under the traditional educational model, the practical link has many deficiencies: the class hours are quite short, students have few opportunities for hands-on operation; the content is full of many verification experiments, lacking comprehensive, inquiry-based, and innovative training methods. There is a shortage of resource support—due to insufficient funds, equipment is limited, and high-performance computing platforms and professional guidance teams are difficult to meet the needs effectively. The curriculum arrangement cannot be connected with cutting-edge scientific research and industrial dynamics, and the existing cases are outdated, resulting in students' practical operation skills not being aligned with the corresponding industrial skills.

2.3. Single teaching method

Traditional classroom teaching mostly adopts the one-way indoctrination form of "teacher lecture + PPT presentation", lacking the design of interactive links, making it difficult to fully stimulate students' learning initiative. For the highly abstract conceptual system of molecular dynamics theory, if only the cramming teaching method is used, students are prone to a sense of difficulty. The understanding of core knowledge is inevitably superficial; there are few opportunities for classroom interaction, and teachers' ability to observe students' learning status and provide personalized guidance is limited. This "one-size-fits-all" educational method ignores the needs of individual differences, leading to reduced learning enthusiasm and poor results for students with weak foundations.

3. Important value of teaching reform for the molecular dynamics course in universities

3.1. Conducive to consolidating students' theoretical foundations

Through improving the curriculum system and updating the educational model, teaching reform can enable students to have a deeper understanding of the core theories of molecular dynamics. Adopting advanced educational resources and integrating the latest research results to update textbook content can not only expand the breadth of students' knowledge but also keep them abreast of the cutting-edge of disciplinary development, gradually forming a systematic knowledge structure. Strengthening the design of experimental links and adding comprehensive and inquiry-based practical projects allows students to deepen theoretical cognition and improve the ability to solve practical problems during hands-on operations [2]. Comprehensive teaching reform helps consolidate students' basic theoretical foundation, enhances their practical ability to comprehensively apply knowledge to solve problems, and lays a solid foundation for future scientific research or career development.

3.2. Conducive to stimulating students' learning interest

The traditional teaching model is restricted by insufficient stimulation of students' learning interest, while the application of innovative educational concepts can effectively break this constraint by integrating case analysis with project-driven methods. Enhance the application value of the course through specific practical scenarios, establish virtual simulation laboratories and online learning platforms to provide technical support for students' independent inquiry; emphasize students' dominant position, encourage their active participation and proactive thinking in classroom interaction and experimental design, thereby stimulating their internal positive factors, and promoting the development of potential and innovative abilities [3].

3.3. Conducive to adapting to disciplinary development trends

The development of molecular dynamics has made its position prominent in scientific research and industry, and the industry's demand for high-level professional talents in molecular dynamics remains at a high level. In this critical context, university education should make changes, attach importance to the integration of high-quality teaching resources and the transformation of practical teaching methods, enable students to systematically master cutting-edge theoretical knowledge and the latest research methods, help students meet practical problems and various market needs; let students learn the innovative abilities of thinking, criticizing, and improving cooperation. These abilities and technologies are the basic requirements for high-end scientific researchers, and are conducive to the integration and sustainable development of production, education, and research [4].

4. Teaching reform strategies for the molecular dynamics course in universities

4.1. Integrate cutting-edge educational resources to stimulate students' learning interest

The optimization of teaching content is a key link in educational reform. Its essence lies in enhancing the forward-looking, practical, and interactive nature of the curriculum system by integrating and updating high-quality educational resources, thereby arousing students' learning interest. First, update textbook content. Schools should promote textbook updates in many aspects, revise existing textbooks regularly, compile new textbooks, incorporate the latest disciplinary research results and industry practice situations, add content such as emerging simulation methods (e.g., machine learning-assisted molecular dynamics, quantum mechanics-molecular dynamics coupled simulation) and complex system simulations (e.g., biological macromolecule folding, catalyst surface reactions), delete outdated or obsolete content, and ensure that teaching content keeps pace with the disciplinary frontier. Second, actively adopt scientific research resources. Schools can invite experts to give special lectures to introduce the wide application and cutting-edge trends of molecular dynamics in fields such as new energy materials design and drug screening, encourage teachers to transform their own research results into teaching materials, and guide students to participate in some experimental operations to deepen their understanding [5]. Third, integrate online educational resources. Teachers can build a variety of online learning environments with the help of Internet platforms, integrate high-quality online course resources at home and abroad (such as molecular dynamics-related courses on Coursera and Xuetang Online), official tutorials of simulation software, and cutting-edge research papers to provide resource support for students' independent learning. At the same time, set up special forums to enhance communication and interaction, creating an open and inclusive teaching atmosphere. Fourth, optimize the structure of teaching content. Teachers can adopt a three-stage model of "basic theory + cutting-edge progress + practical application" to effectively unify knowledge imparting and ability training. First, form a solid basic theoretical framework, then conduct in-depth discussions on hot research areas, and finally help students practice through typical case analysis, improving the overall effect under the premise of ensuring logical rigor.

4.2. Build a virtual simulation platform to carry out virtual experimental teaching

To address problems such as insufficient resources and poor effects in practical teaching, schools can build a virtual simulation experimental platform to optimize the teaching process and improve the effects of practical teaching. First, build a virtual simulation teaching platform. Schools can use high-performance computing platform clusters to integrate resources such as molecular dynamics simulation software (e.g., GROMACS, LAMMPS, NAMD) and visualization software (e.g., VMD, PyMOL) to construct a comprehensive virtual experimental environment combining theoretical explanation, interactive operation, and data analysis, providing an operable environment for students' various learning activities [6]. Second, design multi-level virtual experimental teaching content. Teachers can set up progressive and hierarchical virtual experimental activities according to students' cognitive laws and development rules. Among them, basic verification experiments mainly focus on the learning of basic theoretical knowledge, such as equilibrium state simulation and energy minimization of simple molecular systems, allowing students to master the basic operation of simulation software; comprehensive design experiments introduce examples of actual engineering scenarios, such as stability simulation of protein molecules and tensile deformation simulation of metal materials, prompting students to use learned knowledge to solve certain difficulties; innovative inquiry experiments allow personalized inquiry and cutting-edge scientific research inquiry, and can guide students to independently design simulation projects, such as performance simulation of new catalysts and interaction simulation between drug molecules and target proteins, thereby stimulating students' motivation to understand the real world and enhancing their research creativity [7]. Third, strengthen the guidance of virtual experimental teaching. Schools should set up a professional virtual experimental teaching guidance team to provide full-process guidance and online and offline guidance services for students. Online, they can respond to students' thinking questions in a timely manner through the platform and deliver a variety of materials online; offline, they can carry out relevant operation exercises with the help of university physical laboratories, prompting students to firmly grasp the essence and improve their practical operation skills [8].

4.3. Innovate classroom teaching methods to deepen the understanding of theoretical knowledge

In the teaching reform work, teachers should abandon the traditional one-way indoctrination teaching model and innovate classroom teaching methods to enhance interactivity, arouse students' sense of subject participation, and deepen their understanding and grasp of theoretical knowledge. First, adopt the case teaching method.

Teachers can select typical cases from scientific research practice or industry applications, such as simulation of ion migration behavior in lithium battery electrode materials, integrate abstract concepts into specific scenarios, and, through group discussions, role-playing, and other forms, encourage students to use learned knowledge to solve practical problems, thereby improving their comprehensive literacy [9]. Second, implement the project-driven learning strategy. Teachers can assign modular assignments around specific tasks, such as "molecular dynamics simulation" and "protein structure prediction", allowing students to complete project tasks in groups, independently search for information, design schemes in teams, conduct simulation operations, and analyze project research results, cultivating students' independent thinking ability, team collaboration spirit, and critical thinking in real scenarios [10]. Third, adopt the flipped classroom teaching model. Teachers can push online materials to students in advance for them to independently preview key content, including micro-lecture videos, literature abstracts, and relevant exercises, thereby making class time valuable, focusing on difficult problem analysis, in-depth discussions, and achievement presentation links, realizing two-way interaction between teachers and students, and improving the overall teaching quality [11]. Fourth, use multimedia technology to assist teaching. Teachers can use animations, videos, visual simulations, and other methods to visualize and materialize abstract content, such as the motion process of micro-particles and the implementation process of simulation algorithms, helping students better understand theoretical knowledge and reduce learning difficulties [12].

4.4. Optimize the teaching evaluation system and dynamically adjust teaching activities

Traditional teaching evaluation mostly relies on final exam results, and this single evaluation form is difficult to comprehensively and objectively reflect students' learning status and development potential [13]. In this regard, teachers should establish a diverse evaluation framework and integrate the process-oriented concept, which is the key to improving educational quality. First, build a comprehensive indicator framework covering the entire learning process. Teachers should combine academic achievements with learning results, including pre-class preview investment, classroom interaction frequency, group collaboration results, and virtual experimental operation skills, and ensure that process-oriented elements account for more than half of the total score, thereby comprehensively assessing students' independent inquiry ability, hands-on practical creation ability, and ability to analyze and question problems [14]. Second, enrich evaluation methods. Teachers should combine online and offline methods for evaluation, comprehensively consider data support collected from various forms such as teacher guidance, peer assistance, and personal thinking, and establish a regular reporting mechanism to continuously improve the evaluation scheme. Third, establish a teaching feedback mechanism. Fully solicit opinions from teachers and students during the research stage, adjust teaching activities according to the research results, optimize teaching content and teaching methods, and improve teaching quality. At the same time, teachers should improve the result utilization system, making scores a driving force for students' growth rather than a standard tool for distinguishing strengths and weaknesses, thereby driving the steady improvement of overall teaching quality [15].

5. Conclusion

In summary, the teaching reform of the molecular dynamics course in universities is an inevitable requirement to adapt to disciplinary development trends and cultivate high-quality innovative talents. In the teaching process, schools should integrate cutting-edge educational resources, build virtual simulation platforms, innovate classroom teaching methods, and optimize the teaching evaluation system to improve the quality of course teaching, stimulate students' learning interest and initiative, and cultivate their theoretical foundations, practical abilities, and innovative thinking. With the continuous development of disciplines and the continuous progress of teaching technology, the teaching reform of the molecular dynamics course should be continuously deepened, and more scientific and effective teaching models should be continuously explored to transport more high-quality professional talents to the scientific research field and industry, promoting disciplinary development and industrial upgrading.

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References

[1] Yuan R, Zhang HX, Du PL, 2024, Application of Molecular Dynamics Simulation in Organic Chemistry Teaching. Guangzhou Chemical Industry, 52(23): 197–199.

[2] Lu CY, Xu XY, Yuan ZY, et al., 2024, Application of Molecular Dynamics Simulation in Physical Chemistry Teaching: Wettability of Solid Surfaces. Chemical Engineering Design Communications, 50(11): 79–81 + 85.

[3] Xu ZM, Wang YB, Liu ZH, et al., 2025, Experimental Design for Computational Materials Science and Computational Chemistry Courses Based on the Bohrium Scientific Computing Cloud Platform. University Chemistry, 40(3): 36–41.

[4] Lü GJ, Zhao SJ, Qiao JC, 2024, Interpretation of the Application of Molecular Dynamics Simulation in the Viscoelastic Mechanics of Metallic Glasses from a Teaching Perspective. Mechanics in Engineering, 46(6): 1298–1302.

[5] Xu ZM, Zheng MB, Liu ZH, et al., 2024, Project-Based Experimental Design for Computational Chemistry and Computational Materials Science: Molecular Dynamics Simulation of Organic Electrolytes for Lithium-Ion Batteries. Chinese Journal of Chemical Education (Chinese & English), 45(6): 91–98. https://doi.org/10.13884/j.1003-3807hxjy.2023060009

[6] Jiao B, Wang Y, Zhao N, 2024, Application of Molecular Dynamics Simulation Technology in Materials Mechanics Teaching. The Guide of Science & Education, 2024(8): 50–52. https://doi.org/10.16400/j.cnki.kjdk.2024.8.017

[7] Miao XK, Xie JQ, Yang WL, et al., 2024, Application of Molecular Dynamics Simulation in Medical Microbiology Experimental Teaching. Basic Medical Education, 26(2): 136–139. https://doi.org/10.13754/j.issn2095-1450.2024.02.10

[8] Liu SL, 2024, Application of the SPC/E Water Model in Molecular Dynamics Teaching Experiments. University Chemistry,39(4): 338–342.

[9] Hua CY, 2022, Integration of Science and Education to Promote Excellent Talent Training——Molecular Dynamics Virtual Simulation Teaching. Research and Exploration in Laboratory, 2022, 41(05): 248-252. https://doi.org/10.19927/j.cnki.syyt.2022.05.051

[10] Qu JL, Zhou LX, Sui G, et al., 2020, Undergraduate Teaching Experiment of Molecular Dynamics Simulation on the Glass Transition Process of Polymers. Polymer Bulletin, 2020(3): 63–66. https://doi.org/10.14028/j.cnki.1003-3726.2020.03.009

[11] Tao J, Xu YJS, Shen YZ, et al., 2025, Teaching Exploration and Practice for Outstanding Engineers—Taking the Teaching of Wettability Characteristics of Solid Material Surfaces as an Example. University Education, 2025(8): 54–60.

[12] Chen L, Wang Q, Xiong L, et al., 2024, Strategy for the In-Depth Integration of Simulation Calculation and Curriculum Ideology and Politics in Teaching—Taking the Teaching of the Foundation of Materials Science and Engineering Course as an Example. Jiangxi Chemical Industry, 40(4): 107–112. https://doi.org/10.14127/j.cnki.jiangxihuagong.2024.04.016

[13] Huang H, Cai B, Wang MX, 2024, Exploration of an Innovative Talent Training Model for Physics Driven by Molecular Dynamics Simulation Technology. University Education, 2024(16): 71–74.

[14] Zhou JH, Li N, Li H, et al., 2023, Molecular Dynamics Simulation of Methyl Methacrylate-Butyl Acrylate Copolymer. Leather Science and Engineering, 2023, 33(3): 7–11. https://doi.org/10.19677/j.issn.1004-7964.2023.03.002

[15] Shao K, 2021, Research on the Thermal Transport Properties of Low-Dimensional Carbon Nanomaterials by Molecular Dynamics Simulation, thesis, Beijing Institute of Petrochemical Technology. https://doi.org/10.27849/d.cnki.gshyj.2021.000059