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A Preliminary Study on the Construction of a Knowledge Graph for a *Computational Materials Science* Course

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Abstract: As an interdisciplinary course, *Computational Materials Science* is plagued by pain points and challenges such as abstract and complex content and fragmented knowledge points, which bring heavy learning burdens on students and bring difficulties for teachers in teaching. Featuring systematization, visualization and correlation of knowledge points, knowledge graphs can effectively support in-depth interaction and systematic learning among knowledge points. Based on the practical process of independently building the knowledge graph for *Computational Materials Science* by the course team, this paper systematically introduces the implementation process, including sorting out knowledge points, constructing logical correlations, embedding resources and deploying the knowledge graph, so as to provide references for the digital-intelligent teaching reform of other courses.

Keywords: Computational materials science; Knowledge graph; Course construction

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1. Introduction

In recent years, with the rapid development of new digital and information-based technologies, the state has continuously promoted the in-depth development and reform of digital-intelligent education at the strategic level. From the development goal of "Three-Comprehensiveness, Two-Highs and One-Great" proposed in the *Action Plan for Education Informatization 2.0* in 2018, to the full launch of the *National Education Digitalization Strategic Initiative* in 2022, and further to educational reform documents such as the *Outline for the Construction Plan of a Powerful Country in Education* and the *Nine-Department Opinions on Digitalization* in 2025, the state has continuously promoted the in-depth integration of artificial-intelligence technologies with education and teaching from the policy dimension, and driven systematic innovation in curriculum systems and teaching methods. Against such a background, how to construct curriculum knowledge structures and improve teaching efficiency with digital-intelligent technologies has become an important task for teachers to carry out teaching reform.

Computational Materials Science is an emerging interdisciplinary course integrating materials science,

physics, chemistry, mathematics and computer science. Adopting numerical simulation and calculation as means, it reveals the structure-property relationships of materials from atomic-electronic scale to mesoscopic and macroscopic scales. It serves as an indispensable core method for modern materials research [1]. Due to complicated course content, abstract theories, numerous formula derivations, and complex software operations, students generally encounter difficulties in understanding, fragmented knowledge, and disconnection between theory and practice in the learning process. Meanwhile, although a large number of scattered teaching videos and operation tutorials on the Internet have lowered the entry threshold, they have further aggravated the fragmentation of knowledge systems, making it hard for students to form complete, systematic and coherent knowledge frameworks. How to help students build systematic knowledge systems from massive fragmented information and improve their knowledge-transfer ability and problem-solving ability constitutes the core challenge for the teaching of *Computational Materials Science*.

The knowledge graph is a concept put forward by Google in 2012, and it has been rapidly and widely applied in fields such as intelligent search and personalized recommendation. Its essence lies in the idea that knowledge points do not exist in isolation; instead, semantic networks realize correlations among knowledge points and in-depth interaction with external resources, which meets the requirements for in-depth learning of complex professional knowledge in higher education [2]. In recent years, knowledge graphs have been gradually applied in university curriculum construction, such as *Circuit and Electronics* from Harbin Institute of Technology [3], *Advanced Language Programming* from Beijing University of Technology [4], *Fundamentals of Chemical Engineering Technology* from Tianjin University [5], *Medicinal Plant Cultivation* from Shanxi Agricultural University [6], and *Inorganic Chemistry Experiment* from Hunan Institute of Engineering [7]. Among materials-related courses, existing courses with knowledge-graph construction include *Mechanics of Materials* from Beihang University [8], *Textile Materials Science* from Wuhan Textile University [9], *Packaging Materials Science* from Guangxi University [10], and *Metal Materials and Heat Treatment* from North Minzu University [11]. Nevertheless, up to now, the construction of knowledge graphs for the course *Computational Materials Science* is still in a blank state.

Based on the above background, this paper conducts systematic research on the construction of the knowledge graph for the *Computational Materials Science* course, clarifies construction ideas, sorts out key technologies, summarizes practical features and construction difficulties. It is expected to finally form a replicable and promotable construction scheme for curriculum knowledge graphs, so as to promote innovation in the teaching mode of *Computational Materials Science* and improve talent-cultivation quality.

2. Overview of the *Computational Materials Science* course

Computational Materials Science is a compulsory major course or core elective course for senior undergraduates and postgraduates majoring in materials science and engineering, physics and other related majors in universities. Taking computer simulation and calculation as a tool, the course studies key scientific issues such as the microelectronic structure, thermodynamic properties, dynamic behaviors and optical performances of materials. It acts as a core supporting technology for modern materials research to evolve from “trial-and-error-based R&D” toward “high-throughput design, prediction and screening”. The course covers basic theories including quantum mechanics, solid-state physics and crystal structures, as well as mathematical knowledge such as numerical algorithms and optimization methods. Meanwhile, it requires students to master the operation of at least one mainstream materials-simulation software, and possess practical

capabilities including modeling, parameter setting, task submission, result analysis and data visualization. Therefore, the course integrates theoretical, abstract, practical and engineering attributes, and puts forward high requirements for students' comprehensive capabilities.

From the perspective of current teaching status, the teaching of *Computational Materials Science* faces multiple practical dilemmas. First, the course features complicated content, massive knowledge, and high abstraction. Core concepts such as fundamentals of quantum mechanics, density functional theory, molecular dynamics, Monte-Carlo method, band theory, density of states, phonon spectra, structural relaxation and transition-state search are highly theoretical and difficult to understand, making it hard for students to establish intuitive physical pictures. Second, the textbook system is imperfect. As a fast-developing interdisciplinary subject, *Computational Materials Science* has a limited number of textbooks at home and abroad. Different textbooks vary greatly in emphases: some focus on theoretical derivation while others stress software operation. None of them can fully fit the teaching objectives, scientific-research characteristics, and students' foundations at this university. Third, the problem of knowledge fragmentation is prominent. With increasingly abundant online-learning resources, students can obtain a large number of software-operation videos, short explanatory videos for knowledge points and scattered notes via the Internet. Although such resources facilitate quick entry into the subject, they lack systematicness, logic and coherence. Students tend to stay at the superficial-learning level of "clicking the mouse and modifying parameters", failing to understand the essence, scope of application and result reliability of methods, and cannot form complete knowledge systems. Fourth, theoretical teaching is seriously disconnected from software practice. Classroom teaching mostly focuses on theoretical explanation, while software operation is largely left for students to learn by themselves after class. Teachers can hardly provide full-process tracking and guidance. As a result, the common phenomenon occurs that "students understand theories but cannot perform calculations, or they can operate software without understanding theories". Given the above characteristics of the *Computational Materials Science* course, traditional teaching modes can hardly meet the talent-cultivation demands for innovation-oriented talents in the new era. Intelligent and digital teaching tools are urgently needed to reconstruct knowledge systems and improve teaching effectiveness.

3. Necessity of constructing the knowledge graph for *Computational Materials Science*

For beginners, *Computational Materials Science* features numerous knowledge points, complicated relationships and diverse hierarchies. Without a systematic system, students are highly likely to fall into a vicious cycle of "forgetting previous content after learning new ones, forgetting theories after learning operations". The core value of *Computational Materials Science* lies in "guiding computational simulation with physical theories and revealing the essence of material properties through simulation results". In actual teaching, theories and practical operations are relatively separated. Students cannot figure out the theoretical basis and physical significance behind each software parameter and operation, and fail to achieve closed-loop cognition of "theory-model-software-parameter-result". Given the diverse foundations of students, existing teaching cannot satisfy personalized online and offline learning paths for students. To construct a systematic knowledge system, break down barriers between theories and software-practice operations, and support personalized learning paths for students, the construction of a knowledge graph is an inevitable choice. Meanwhile, it fills the gap in knowledge-graph construction for the *Computational Materials Science* course.

4. Training objectives of the *Computational Materials Science* course

To ensure clear orientation and accurate positioning of knowledge-graph construction for talent-cultivation services, clarifying the course training objectives constitutes the primary task. All courses shall build a four-dimensional training-objective system guided by "knowledge as foundation, competence as priority, quality as essence, and ideological-political education as soul", where the four elements progress step-by-step and are organically unified.

First, the knowledge objective serves as the foundation and the prerequisite for realizing competence, quality and ideological-political objectives. Through course learning, students are required to master core principles of *Computational Materials Science*, various computational methods and knowledge of mainstream software, understand disciplinary frontiers and application boundaries, and form complete knowledge frameworks.

Second, the competence objective represents the externalization and application of knowledge objectives and constitutes the core task of course teaching. Through systematic learning, students can skillfully complete simulation and analysis using mainstream software such as VASP, and possess the capabilities to independently design computational schemes, interpret results, and analyze relationships between material structures and properties.

Third, the quality objective is the sublimation of competence, resulting from long-term accumulation of knowledge and competence, and in turn promotes deepened knowledge and improved competence. It is necessary to cultivate students' interdisciplinary-research concept of the trinity of "theory-computation-experi ment", develop rigorous scientific thinking, interdisciplinary-integration concepts and independent-innovation capabilities, as well as standardized scientific-research habits and a realistic and pragmatic scientific attitude.

Fourth, the ideological-political objective provides orientation guidance and runs through the whole process. Students are required to understand China's international status in relevant fields, stimulate their patriotism and dedication to science for the nation, and foster craftsmanship, so as to finally achieve the educational goal of "mastering professional knowledge and practicing the mission of serving the country".

5. General ideas for constructing the curriculum knowledge graph

The construction of the knowledge graph for this course follows the general idea of "knowledge sorting — correlation construction — resource support — platform deployment". The whole process centers on teaching requirements and learning rules to promote graph construction in an orderly manner and guarantee the practicality and usability of the graph.

First, in combination with teaching requirements, comprehensively decompose teaching contents, accurately sort out and screen core knowledge points of the course to ensure pertinence, practicality and effectiveness.

Second, deeply analyze internal correlations among knowledge points, clarify hierarchical structures and pre-dependency relationships, break down isolation barriers between knowledge points, and build clear logical knowledge frameworks.

Third, bind self-compiled textbook texts, original videos, scientific-research cases and a small number of high-quality external online resources carrying knowledge points to corresponding knowledge points, so as to realize the organic integration of knowledge points and resource packages.

Finally, import teaching resources into the Rain Classroom module of the Xuetang Online platform to

build a logically rigorous, hierarchically clear curriculum knowledge graph adapted to teaching-and-learning requirements, and finish the digital-intelligent construction of this course.

6. Implementation process for constructing the knowledge graph in the course

Built on the Rain Classroom platform of Xuetang Online and leveraging the knowledge-graph-construction access granted by the university, the knowledge graph for this course is systematically implemented in three phases.

(1) Phase 1: Systematic Sorting of Curriculum Knowledge Points

Based on self-compiled textbooks, self-compiled teaching courseware, original teaching-and-operation videos and scientific-research cases, combined with this university's teaching syllabus and scientific-research orientations, the whole course is divided into five major knowledge units: Basic Theories of Computational Materials Science, Molecular-and-Crystal Computational Theories, Molecular Dynamics and First-Principles Methods, Material-Structure Prediction and Property Calculation, as well as Computer Practice and Scientific-Research Cases. Further subdivision yields 98 learning units. A total of 127 core knowledge points are sorted out, matched with 43 original teaching videos, 10 scientific-research cases and abundant text and PPT resources, forming a complete list of knowledge points and a resource library.

(2) Phase 2: Construction of Internal Correlations Among Knowledge Points

Knowledge-point correlation lies at the core of the knowledge graph. This course adopts textbook chapters as first-level nodes, learning units as second-level nodes, and specific knowledge points as bottom-level nodes to build a hierarchical knowledge network. Key relationships are clarified: dependency relationships between pre-knowledge points and subsequent knowledge points, supporting relationships between theoretical knowledge points and methodological knowledge points, application relationships between methodological knowledge points and software practice operations, and inclusion relationships between core concepts and sub-concepts. Taking density functional theory as an example, the following logical chain is constructed: *Fundamentals of Quantum Mechanics → Hohenberg-Kohn Theorems → Kohn-Sham Equations → Exchange-Correlation Functionals → Pseudopotential Plane-Wave Method → Structural Relaxation → Implementation via VASP Software → Result Analysis*, forming a complete correlation chain from theories to methods and further to practical operations.

(3) Phase 3: Platform-Oriented Construction of the Knowledge Graph

Import knowledge points attached to resource packages, including texts, PPTs, videos, and cases, onto the Rain Classroom platform in hierarchical order to finish visual construction of the knowledge graph. The completed knowledge graph supports visual display of knowledge points, automatic generation of learning paths, quick jumps among knowledge points, real-time collection of learning data, intelligent diagnosis of weak knowledge points, and personalized resource recommendation. It ultimately forms a systematic, visual, intelligent and dynamically-updatable knowledge graph for the *Computational Materials Science* course (**Figure 1**).

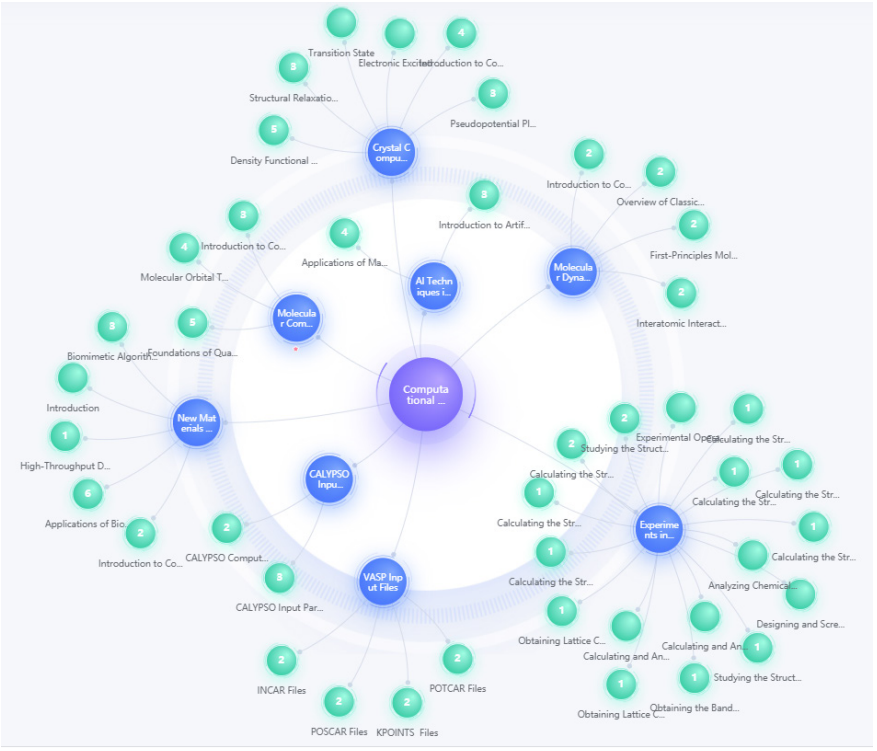

Figure 1. Knowledge Graph for the *Computational Materials Science* Course.

7. Characteristics of the constructed knowledge graph for the *Computational Materials Science* course

Rooted in the reality of this university, highlighting scientific-research advantages and prioritizing original content, the constructed knowledge graph for this course presents two distinct characteristics.

First, it is grounded in the university's scientific-research reality and highlights pertinence and practicality. Core members of the course team focus their research on nonlinear optical crystals and electrocatalytic CO_2 reduction. Their research mainly covers electronic and atomic scales and centers on the application of density functional theory. Knowledge points closely related to these research orientations are screened, practical-operation essentials for the two research fields are sorted out, forming an integrated "theory-scien tific-research-practice" chain. It fits the university's scientific-research characteristics and realizes seamless connection between teaching and scientific research.

Second, it adheres to content originality and builds diversified knowledge-resource systems. Core knowledge-point contents of the knowledge graph derive from self-compiled textbooks, in-class PPTs and original teaching videos of the team, which are highly adapted to the university's teaching reality and students' foundations and guarantee originality and exclusivity of the knowledge system.

8. Conclusion

In response to national requirements for digital-intelligent education, the course team has preliminarily built the knowledge graph for the *Computational Materials Science* course relying on the Rain Classroom platform of Xuetang Online. It realizes the systematization and visualization of curriculum knowledge points, provides

personalized and diversified learning paths and sufficient learning resources for students studying this course, builds a complementary mode combining offline classroom teaching and online learning, and effectively improves learning effectiveness. Meanwhile, it offers references for the construction of digital-intelligent knowledge graphs. Of course, knowledge-graph construction is not a one-off project but a long-term process of continuous iteration and dynamic optimization. In the future, the course team will test the application effects of the knowledge graph in actual teaching, continuously update knowledge points according to students' learning data, teaching feedback and the latest scientific-research achievements, keep promoting the optimization and application of the knowledge graph, and give full play to its core supporting role in course teaching and learning.

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Disclosure statement

The authors declare no conflict of interest.

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