CyberMAGICS: Cyber Training on Materials Genome Innovation for Computational Software for Future Engineers

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Abstract

Computing landscape is evolving rapidly. Exascale computers have arrived, which can perform 10^{18} mathematical operations per second. At the same time, quantum supremacy has been demonstrated, where quantum computers have outperformed these fastest supercomputers for certain problems. Meanwhile, artificial intelligence (AI) is transforming every aspect of science and engineering. A highly anticipated application of the emerging nexus of exascale computing, quantum computing and AI is computational design of new materials with desired functionalities, which has been the elusive goal of the federal materials genome initiative. The rapid change in computing landscape resulting from these developments has not been matched by pedagogical developments needed to train the next generation of materials engineering cyberworkforce. This gap in curricula across colleges and universities offers a unique opportunity to create educational tools, enabling a decentralized training of cyberworkforce.

To achieve this, we have developed training modules for a new generation of quantum materials simulator, named AIQ-XMaS (AI and quantum-computing enabled exascale materials simulator), which integrates exascalable quantum, reactive and neural-network molecular dynamics simulations with unique AI and quantum-computing capabilities to study a wide range of materials and devices of high societal impact such as optoelectronics and health. As a single-entry access point to these training modules, we have also built a CyberMAGICS (cyber training on materials genome innovation for computational software) portal, which includes step-by-step instructions in Jupyter notebooks and associated tutorials, while providing online cloud service for those who do not have access to adequate computing platform. The modules are incorporated into our open-source AIQ-XMaS software suite as tutorial examples and are piloted in classroom and workshop settings to directly train many users at the University of Southern California (USC) and Howard University—one of the largest historically black colleges and universities (HBCUs), with a strong focus on underrepresented groups. In this paper, we summarize these educational developments, including findings from the first CyberMAGICS Workshop for Underrepresented Groups, along with an introduction to the AIQ-XMaS software suite. Our training modules also include a new generation of open programming languages for exascale computing (*e.g.*, OpenMP target) and quantum computing (*e.g.*, Qiskit) used in our scalable simulation and AI engines that underlie AIQ-XMaS.

Our training modules essentially support unique dual-degree opportunities at USC in the emerging exa-quantum-AI era: Ph.D. in science or engineering, concurrently with MS in computer science specialized in high-performance computing and simulations, MS in quantum information science or MS in materials engineering with machine learning. The developed modular cyber-training pedagogy is applicable to broad engineering education at large.

1. Introduction

***Nexus of exascale computing, quantum computing and AI*:** Computing landscape is evolving rapidly. Exascale computers have arrived, which can perform 10^{18} mathematical operations per second (https://www.top500.org) [1]. At the same time, quantum supremacy has been demonstrated, where several quantum computers have surpassed the computing power of these fastest supercomputers for selected problems [2, 3]. Meanwhile, artificial intelligence (AI) is transforming every aspect of science and engineering [4, 5], with the entire hardware and software stack tuned to AI [6]. We are one of the 10 initial simulation users of the forthcoming exaflop computer, Aurora, under the Aurora Early Science Program (ESP) award entitled "Metascalable layered materials genome" [1].

***Materials genome and future manufacturing*:** A prime testbed of the emerging nexus of exascale computing, quantum computing and AI is the materials genome initiative (MGI) [7]. In MGI, informatics is applied to design new materials significantly faster than the conventional trial-and-error approach, thereby revolutionizing clean energy, national security and human welfare. Recognizing the need for developing cyberinfrastructure for MGI, U.S. Department of Energy (DOE) has established computational materials science (CMS) centers. One of the first CMS centers is MAGICS (Materials Genome Innovation for Computational Software) at USC. MAGICS has developed a suite of open-source software for use by a broad community of not only materials scientists but also physicists, chemists, biologists and engineers [8-13]. For example, the open-source MAGICS software forms the basis of our future manufacturing project, which develops a transformative manufacturing platform for quantum material architectures using a cybermanufacturing approach, which combines AI, robotics and predictive simulation for the automated and parallel assembly of multiple two-dimensional (2D) materials into complex three-dimensional (3D) structures.

***Challenge—materials cyberworkforce development*:** While materials genome at the exa-quantum-AI nexus promises to advance broad scientific and engineering areas including cybermanufacturing, it poses a tremendous challenge of training a new generation of urgently-needed cyberworkforce, who innovatively combine exascale computing, quantum computing and AI to address Grand Challenge problems in materials genome—a daunting task that cannot be served by traditional educational structures.

Solution—CyberMAGICS (cyber training on materials genome innovation for computational software) infrastructure and course modules*:** To meet this educational challenge, our CyberMAGICS project trains a new generation of materials cyberworkforce who will solve challenging materials genome problems through innovative use of advanced cyberinfrastructure at the exa-quantum-AI nexus. We develop and disseminate training modules for ***a new generation of quantum materials simulator named AIQ-XMaS (AI and quantum-computing enabled exascale materials simulator); see Fig. 1. Based on the MAGICS software suite, AIQ-XMaS integrates exascalable quantum [8, 14], reactive [9] and neural-network [15] molecular dynamics (MD) simulations with unique AI and quantum-computing capabilities to design a wide range of materials. CyberMAGICS training modules are integrated into our open-source AIQ-XMaS software as tutorial examples. To make the training modules easily accessible, we are developing a CyberMAGICS portal as a single access point for all AIQ-XMaS software along with step-by-step tutorial examples and associated lecture notes. We pilot the CyberMAGICS training modules in classroom setting at USC and Howard. CyberMAGICS also brings exascale and quantum computing to classrooms—in addition to simulation and AI,

training modules cover a new generation of open programming languages for exascale computing (*e.g.*, OpenMP target offload) and quantum computing (*e.g.*, Qiskit). To further train broader users, we organize ***CyberMAGICS training workshops with a strong focus on underrepresented groups***.

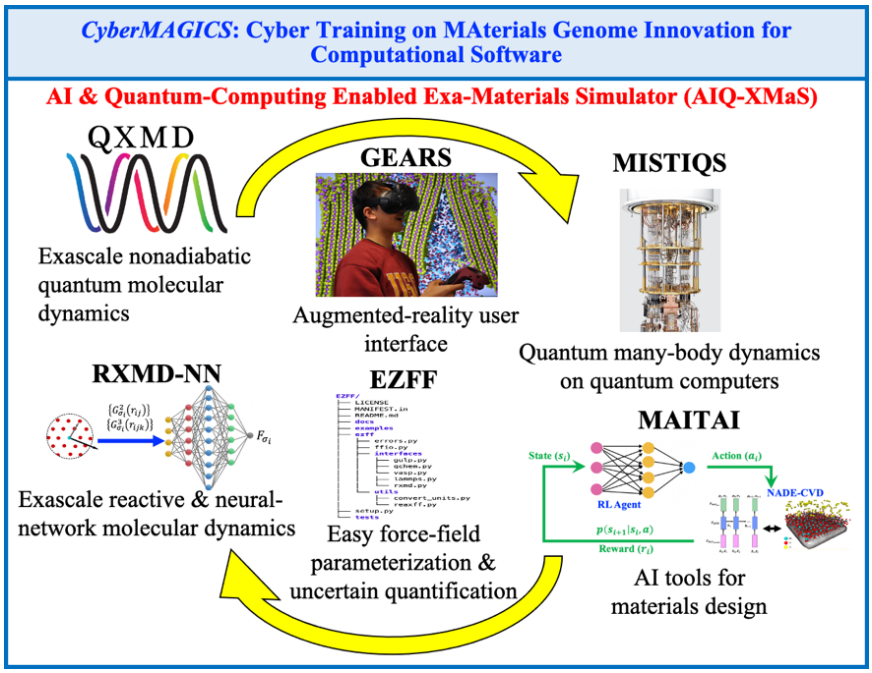

Fig. 1 | CyberMAGICS software: We develop and disseminate training modules on the next generation of quantum materials simulator named AIQ-XMaS (AI and quantum-computing enabled exa-materials simulator).

In the following sections, we provide detailed description of the CyberMAGICS project.

2. CyberMAGICS Training Modules

We are developing a CyberMAGICS portal (https://cybermagics.netlify.app) as a single-access point not only to the AIQ-XMaS software suite but also to the cybertraining modules to be developed as tutorial examples. The following describes key features and representative applications of AIQ-XMaS software components.

***QXMD (https://github.com/USCCACS/QXMD)*:** Scalable software [8] for nonadiabatic quantum molecular dynamics (NAQMD) simulations [16, 17] of coupled electron-lattice dynamics for computational characterization of device performance. Quantum molecular dynamics (QMD) simulations follow the trajectories of all atoms while computing interatomic forces quantum mechanically from first principles in the framework of density functional theory (DFT). To study photoexcitation dynamics, NAQMD simulations describe electronic excited states within the linear response time-dependent density functional theory (LR-TDDFT) and transitions between the excited states using a surface-hopping approach. ***Representative applications*:** QXMD has been used to study ultrafast photoexcitation dynamics in 2D materials [18, 19], photocarrier dynamics in solar cells involving 6,400 atoms [20], sustainable hydrogen production on demand from water involving 16,611 atoms [21], and ferroelectric topological structures such as skrmions for future ultralow-power electronics, *i.e.*, polar topotronics (Fig. 2) [22].

***RXMD-NN (https://github.com/USCCACS/RXMD)*:** Scalable reactive molecular dynamics (RMD) [9] and neural-network quantum molecular dynamics (NNQMD) [22-25] simulations to accurately simulate quantum-mechanical phenomena at a fraction of computing time compared to QMD. RMD describes formation and breakage of chemical bonds using bond order theory and charge transfer based on a charge-equilibration scheme [26]. We have implemented a new polarizable reactive force-field (ReaxPQ) model with improved accuracy in describing polarizable media under electric field [27]. NNQMD simulations based on machine learning (ML) could revolutionize atomistic modeling of materials with quantum-mechanical accuracy at a drastically reduced computational cost. ***Representative applications*:** RXMD-NN has been used for computational synthesis of 2D materials based on chemical vapor deposition (CVD) [28], exfoliation [29] and novel nanofluidic folding [30], and optical and mechanical switching of polar topotronics (Fig. 2) [22, 25].

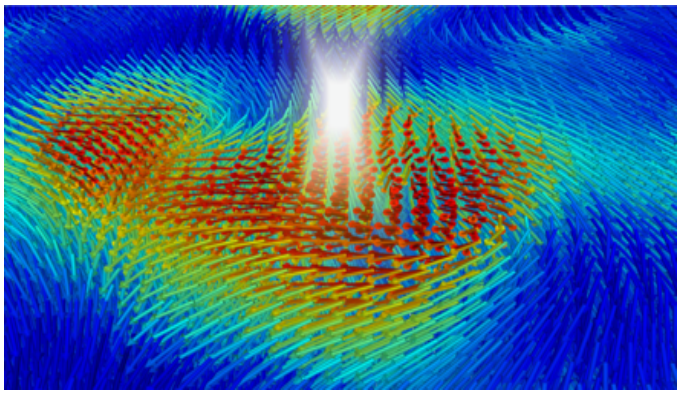

Fig. 2 | Polar topotronics application of our software: Multiscale NAQMD and NNQMD simulations reveal photo-switching of ferroelectric topological structures in $PbTiO_3/SrTiO_3$ hetero-stack.

***EZFF (https://github.com/USCCACS/EZFF)*:** Open-source software for easy force-field development and novel Pareto-frontal uncertainty quantification (UQ) [10]. Construction of high-quality interatomic force fields is a critical first step in performing accurate MD simulations, but the lack of easy software to use has thus far prohibited broader adoption of this critical technology. EZFF is a lightweight Python library for force-field parameter optimization based on multi-objective genetic algorithm (MOGA) [31]. Furthermore, Pareto optimal front in MOGA is used for UQ of quantities of interest [31].

***MAITAI (https://magics.usc.edu/mlaisoft)*:** Materials Informatics Technology enabled by AI, including reinforcement learning (RL) [32] and active learning (AL) [33] to optimize nano-architectures, and deep generative models to find transition pathways [34]. In a manner similar to how AI plays a board game of Go, we use a RL model to design a wide range of optimal nanostructures (*e.g.*, 2D material kirigami) and growth conditions (*e.g.*, temperature control) to achieve desired properties such as large stretchability and minimal defect density. Our AI model combines: (1) RL agent to design patterns; and (2) convolutional neural network-based dynamic model of patterned materials, which are trained by MD simulation data (Fig. 3) [32].

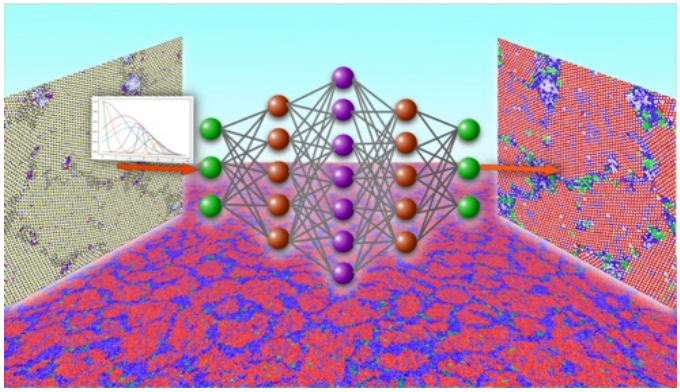

Fig. 3 | Machine learning (ML) approach to layered materials: Feedforward neural network classifies metallic and semiconducting phases as well as defects.

MISTIQS (https://github.com/USCCACS/MISTIQS)*:** Quantum many-body dynamics simulations on emerging quantum computers such as IBM Q and Rigetti Aspen [11, 12, 35, 36]. We will re-architect MISTIQS in a way easily extensible to other problems and quantum languages/circuits. Quantum computing will be mirrored by exascale simulations on an exaflop computer to assess quantum supremacy. We are developing: (1) ***AI-inspired domain-specific quantum compilers to address the fundamental limitation of the noisy intermediate-scale quantum (NISQ) computing technology—environmental noise—by reducing the size and depth of quantum circuits, thereby extending the spatiotemporal scales of simulations within the NISQ fidelity budget [35]; and (2) ***hidden quantum-dynamics learner***, in which an AI model on a classical supercomputer reconstructs the ground-truth quantum dynamics from noisy measurements in quantum circuits [36]. ***Representative application—quantum materials on demand*:** MISTIQS has been used to study ultrafast control of emergent functionality using electromagnetic radiation in 2D materials. In a recent experimental study, emergent magnetism was observed from all nonmagnetic elements in single-layer, Re-doped $MoSe_2$ [37], and MISTIQS simulations showed tunability of 2D magnetization by THz pulse [11].

***GEARS (https://github.com/USCCACS/GEARS)*:** GEARS (Game-Engine-Assisted Research platform for Scientific computing) allows users to develop and interactively perform simulations and experiments in immersive and interactive virtual reality (VR) environment [13]. To enhance the user interface of GEARS, we have acquired a multi-user, mixed-reality (MR) capability under a Microsoft Mixed-Reality Academic Seeding Program. We will use MR-enhanced GEARS to interact with simulations and experiments on-the-fly, while viewing actual physical systems in augmented reality (AR). GEARS is linked to the widely used MD simulation engine, LAMMPS (https://www.lammps.org), with which we demonstrated real-time simulation involving 500,000 atoms within VR.

***Software and training-module dissemination*:** Our software-development workflow is based on industry-standard best practices such as code versioning, recording and issue tracking, and distributed software development using the Github infrastructure, incorporating unit testing, continuous integration and automated documentation to maintain software quality and usability. We create Singularity image files for the software and distribute them from the portal, Github and Singularity repository hub (https://singularity-hub.org). For those who do not have access to computing platform with compatible build environment and third-party libraries, we will use online cloud services such as Code Ocean (https://codeocean.com) and Docker hub

(https://hub.docker.com) to provide open, easy-to-use and reproducible test environments, as we have done for QXMD and RXMD-NN software.

***Piloting in classrooms*:** We will directly train ~200 students per year in the following courses taught in materials science (MASC), chemical engineering (CHE), physics and computer science (CS). This allows us to collect feedback and improve the module contents. We have considerable experience in developing research products into teaching modules [38]. The courses include: MASC 515 (USC)–Basics of machine learning for materials; MASC 520 (USC)–Mathematical methods for deep learning; MASC 575 (USC)–Basics of atomic simulation of materials; MASC 576 (USC)–Molecular dynamics simulations of materials and processes; PHYS 513 (USC)–Application of quantum computers; PHYS 516 (USC)–Methods of computational physics; CSCI 596 (USC)–Scientific computing and visualization; CSCI 653 (USC)–High performance computing and simulations; CSCI 699 (USC)–Extreme-scale quantum simulations; PHYS 235 (Howard)–Molecular simulation; CHE502 (Howard)–Advanced chemical engineering thermodynamics.

***Bringing exascale and quantum computing to classrooms*:** In addition to simulation and AI software, training modules will also include a new generation of open programming languages for exascale computing (*e.g.*, data parallel C++ [39] and OpenMP target offload [40]) and quantum computing (*e.g.*, Qiskit). While we currently teach hybrid parallel programming integrating MPI for message passing, OpenMP for multithreading, and CUDA for data parallelism on graphics processing unit (GPU) in CSCI 596 and CSCI 653, the new generation of open languages provide unified programming of broader heterogenous accelerators such as tensor processing unit (TPU) and field-programmable gate array (FPGA). This effort will leverage a recent Intel grant entitled "Simulation and machine learning at scale on heterogeneous architectures: bringing DPC++ from Intel exaflop/s computer to classrooms", in which we have converted our data-parallel simulation and ML mini-apps within AIQ-XMaS for the forthcoming exaflop/s supercomputer, Intel Aurora, into hands-on course modules that teach the essence of data parallel C++ (DPC++) programming and performance optimization on heterogeneous architectures.

3. CyberMAGICS Workshop

We organize annual workshops to train students and scientists, with a strong focus on underrepresented groups. We believe that, in addition to software distribution via the CyberMAGICS portal and GitHub repositories, the most effective method of software distribution and training is in-person, hands-on training of cyberinfrastructure users who apply the cyberinfrastructure to their immediate research. Jupyter notebook combined with free online cloud such as Google Colab has gained much attention recently in STEM fields where computer simulation or programming exercises are involved in their curricula [41-43]. Virtual machine, such as Virtual Box (https://www.virtualbox.org) or Parallels (https://www.parallels.com), is another widely adapted technology offering seamless and unified learning experiences for workshop participants (Fig. 4). Therefore, all CyberMAGICS training modules were created using Jupyter notebook or performed on online cloud through web browser (Fig. 5). Each three-day workshop consists of lectures on AIQ-XMaS software components, followed by hand-on training sessions using selected tutorial examples. The training gained in the workshops is augmented with the students discussing their own research goals at the end of the workshop and networking with senior personnel from USC and Howard. In this way, we recruit part of the

workshop alumni to the cyberinfrastructure-contributor community, which further develops cyberinfrastructure.

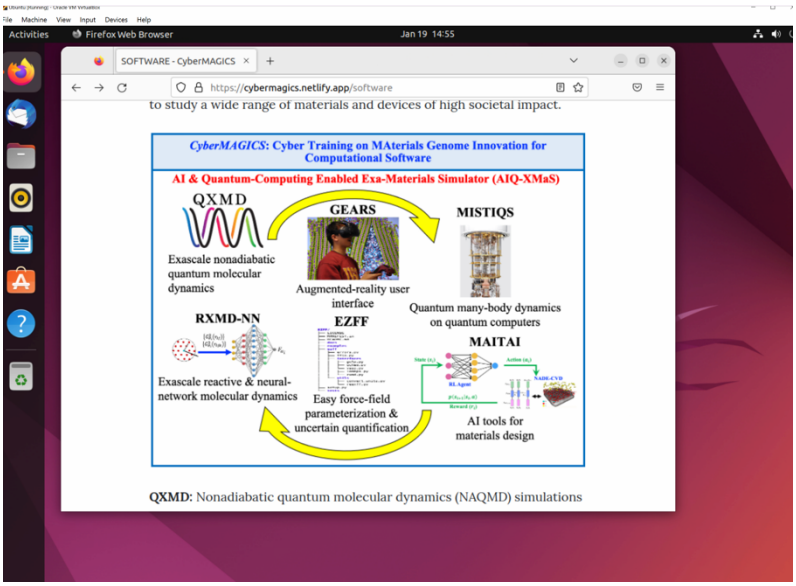

Fig. 4: |Virtual machine (VM) support: Ubuntu Linux VM running on Windows OS. VM allows us to run necessary software to teach workshop participants regardless of their computing platform.

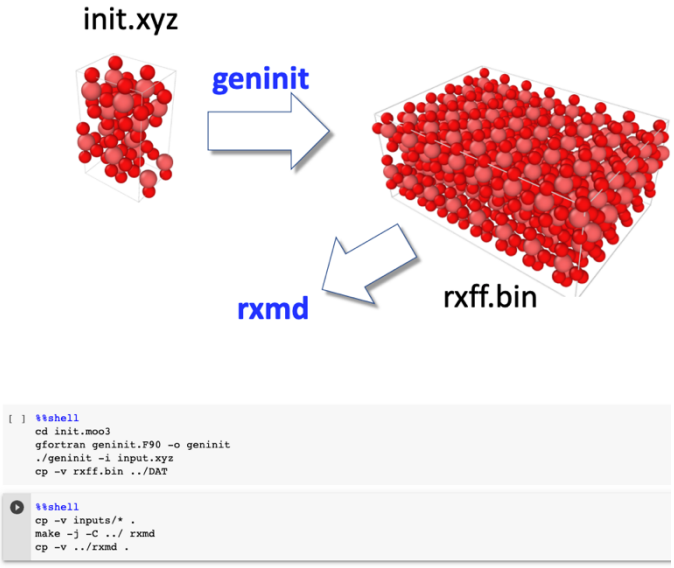

Fig. 5 | Jupyter notebook training module: Snapshot of the RMD hands-on module using Jupyter notebook. Participants were able to go through the training modules on Google Colab from their laptop without any software setup.

The first CyberMAGICS workshop was held virtually on June 30 – July 2, 2022 (Fig. 6). The 36 participants from 16 institutions included graduate students, postdocs and early-career faculty. A large number of participants were female and minority, and the institutions included HBCU and MSI such as Howard University and California State University, Northridge. The schedule included lectures and hands-on training on QMD, RMD and NNQMD simulations, AI for

materials, and quantum computing. On the last day, participants made presentations, followed by extensive discussions.

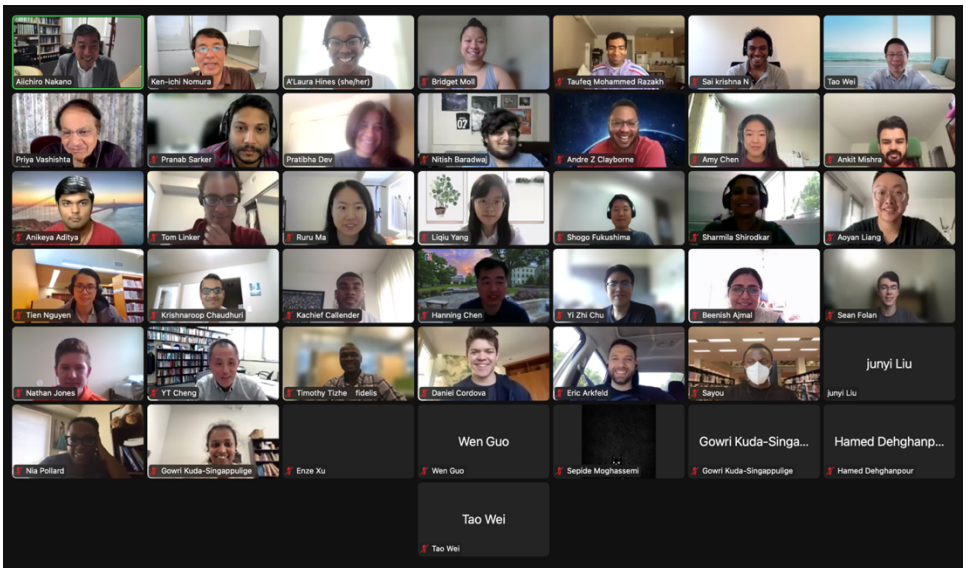

Fig. 6: Participants at the first CyberMAGICS workshop.

The workshop schedule and resources are found at https://cybermagics.netlify.app/workshop-schedule.html.

4. Conclusion and Outlook

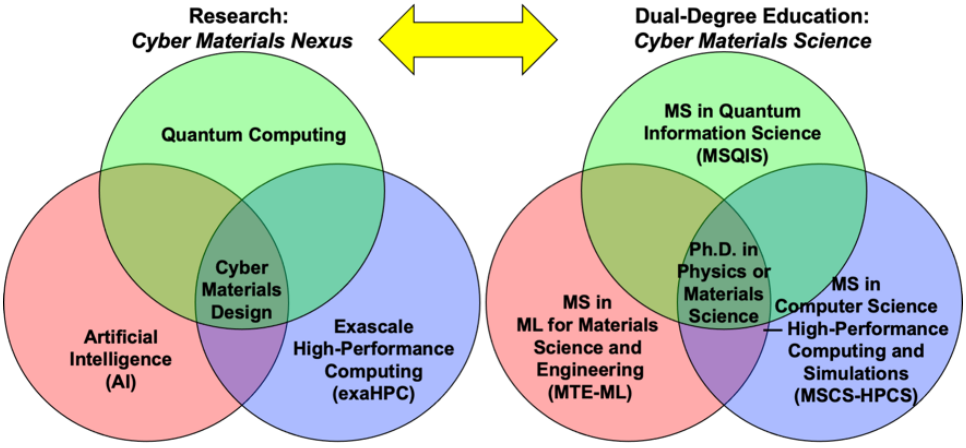

Fig. 7 | Integrated research and education at the exa-quantum-AI nexus: (Left) Materials research at the nexus of exascale & quantum computing and AI. **(Right)** Dual-degree education in cyber materials science combines Ph.D. in physics or materials science with MSCS-HPCS, MSQIS or MTE-ML.

We have developed a modular training approach, CyberMAGICS (cyber training on materials genome innovation for computational software), to educate a new generation of materials cyberworkforce at the new era of exa-quantum-AI nexus. In fact, CyberMAGICS forms a seed to foster the adoption of exa-quantum-AI nexus technologies by a much broader community outside materials science. Students involved in this project at USC receive Ph.D. in materials science or physics, concurrently with MS in computer science specialized in high-

performance computing (MSCS-HPCS), MS in quantum information science (MSQIS) or MS in materials engineering with machine learning (MTE-ML) (Fig. 7), co-supervised by faculty in materials science, physics, chemical engineering and computer science. The dual-degrees opportunities are indeed pursued by Ph.D. students in much broader disciplines including chemistry, biology and a wide range of engineering disciplines.

Acknowledgement

This project was supported by the National Science Foundation, Award OAC-2118061.

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