



A case study: Leveraging reactive molecular dynamics simulations and guided inquiry to foster STEM identity and motivation among college engineering students

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Abstract

This study aims to provide preliminary findings on the integration of reactive molecular dynamics (RMD) simulations with evidence-based instructional strategies to enhance STEM identity and motivation in first-year, first-generation, and low-income college students. Six students from two Hispanic-serving institutions in central California participated in a three-week winter research program, which included 10 instructional modules on materials science topics. The program incorporated hands-on RMD simulation training to deepen students' understanding of chemical reactions at the atomic level. Data collected through pre- and post-surveys and open-ended responses revealed increased STEM identity and motivation, along with improved interest, competence, performance, and recognition in STEM. Additionally, the program demonstrated the potential to enhance students' persistence in STEM learning through positive experiences such as hands-on activities, peer collaboration, and simulations. These findings suggest the winter research program highlighting RMD may strengthen STEM identity and motivation in materials science education.

Introduction

The US Bureau of Labor Statistics [1] reported that the projected growth rate of job openings for material scientists and chemists is 6% between 2022 and 2032, the greatest among all other STEM and non-STEM occupations in US Materials science, which engages students through hands-on

experiments exploring the atomic and molecular structures of materials, has the potential to inspire STEM career interests. However, it remains the least preferred STEM major, with low retention and degree completion rates, particularly among women and underrepresented minorities, including Latinx and African American students [2]. This has contributed to a persistent gap in STEM representation.

STEM identity and motivation have been identified as strong predictors of science achievement and persistence [3–5]. STEM identity often refers to self-perception or self-portrait—how much an individual or others perceive or define them as a “STEM person.” Motivation in learning science refers to students' personal characteristics, including their beliefs, attitudes, and feelings toward STEM or science. Several studies found that STEM identity had the strongest direct effect on predicting students' intentions to persist in physics careers [6–8] STEM identity provides a theoretical lens to better understand the mechanisms by which experiences might influence persistence and career choices. Recent studies emphasize the importance of instruction that fosters STEM identity and motivation through contextualized problem-solving and technology integration. [9, 10] For example, Amelink et al. [11] found hands-on research experiences in nanotechnology and biotechnology improved community

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college students' self-efficacy and career goals. Similarly, other interventions incorporating scientific practices, technology, and collaboration have increased students' STEM interest, retention, and motivation [12, 13].

While increased attention has been given to research on renovating instruction to improve students' achievement and persistence in STEM, little attention has been given to studying the role of students' psychosocial factors, such as motivation, within these efforts. This study seeks to explore the effects of integrating reactive molecular dynamics (RMD) simulations—atomic-level modeling and simulations method that can support computational materials research—with evidence-based instructional strategies on college students' STEM identity and motivation. We assume that these effects, in turn, have the potential to influence students' competence and retention rates in STEM disciplines. To contextualize this research, we conducted a case study with a sample engineering college students participating in a winter research program incorporating RMD training. Our goal was to obtain preliminary findings on whether and to what extent, the program enhanced students' STEM identity development and motivation for learning materials science. Given this purpose, we acknowledge that the small sample size may limit the generalizability of our findings, therefore, a follow-up study with a larger cohort is warranted.

Method

Winter research program

We developed a semester-length co-curricular program to help undergraduate students in engineering majors succeed in a prerequisite chemistry course and other advanced engineering courses. Before implementing the program on a large scale, this study piloted the program with a small group of students during a three-week winter research program. The program consisted of 10 instructional modules covering topics such as the computational design of metal nanoparticles, fracture modeling of glass–ceramics, hydrocarbon combustion, and the computational synthesis of two-dimensional materials. Each module aimed to enhance students' understanding of chemical reactions at the atomic level. Figure 1 provides snapshots of the materials research topics [14–17] integrated into training modules. Recent review articles [18–20] highlight the effectiveness of RMD simulations in college-level chemistry classrooms. Therefore, we believe that the topics proposed in Fig. 1 can enhance students' understanding of atomic-level chemical reactions relevant to engineering and science fields. Two faculty members—one from engineering and the other from STEM education—jointly implemented the program.

The program utilized an asset-based framework to emphasize students' active use of their scientific knowledge, which interacts with their multiple social identities. As part of this process, participants developed graphical representations of their identities, illustrating how different aspects intersect with science or STEM. Guided inquiry-based instruction was incorporated to enhance learning through a structured cycle that actively engaged students in scientific exploration. The cycle included engagement, where students connected with a phenomenon or problem based on their lived experiences; exploration, where they investigated concepts through hands-on activities and collaborative inquiry; explanation, where they analyzed findings and refined their understanding with instructor support; elaboration, where they applied concepts to new contexts and real-world scenarios; and evaluation, where assessments and reflections reinforced learning. By centering students' lived experiences with science, the program aimed to maximize the assets and strengths of underrepresented minority students in their disciplinary development. They shared diverse lived experiences related to chemistry and scientific phenomena, providing a foundation for contextualized learning. These experiences were leveraged to foster scientific inquiry and identity in ways that align with students' existing knowledge and backgrounds. Participants then connected scientific concepts to their academic majors, identifying real-world problems based on their lived experiences. To effectively introduce RMD skills to college students, ReaxFF-based RMD simulations were conducted using commercial software, Amsterdam Modeling Suite with the ReaxFF module [21]. This software provides a full graphical user interface (GUI) on students' laptops and PCs, allowing them to build molecules, run RMD simulations, and analyze results within the GUI this feature increases accessibility for college-level students to model and simulate chemical systems via hands-on activities. Participants monitored real-time step-wise chemical reactions and learned to balance chemical equations by counting reactants and products. They then adjusted the number of reactants to observe the corresponding changes in product formation, gaining an understanding of stoichiometric relationships.

During the program, students followed a structured approach: first, the instructor conducted hands-on practice sessions with step-by-step guidance; second, students engaged in brainstorming to identify scientific problems, formulate inquiries, and establish assumptions; third, students designed simulated materials and performed RMD simulations; fourth, they analyzed the simulation results to validate their assumptions; and lastly, through trial and error, students refined their simulations and models until achieving results that either aligned with their initial assumptions or demonstrated scientific validity. These activities are summarized in Fig. 2.

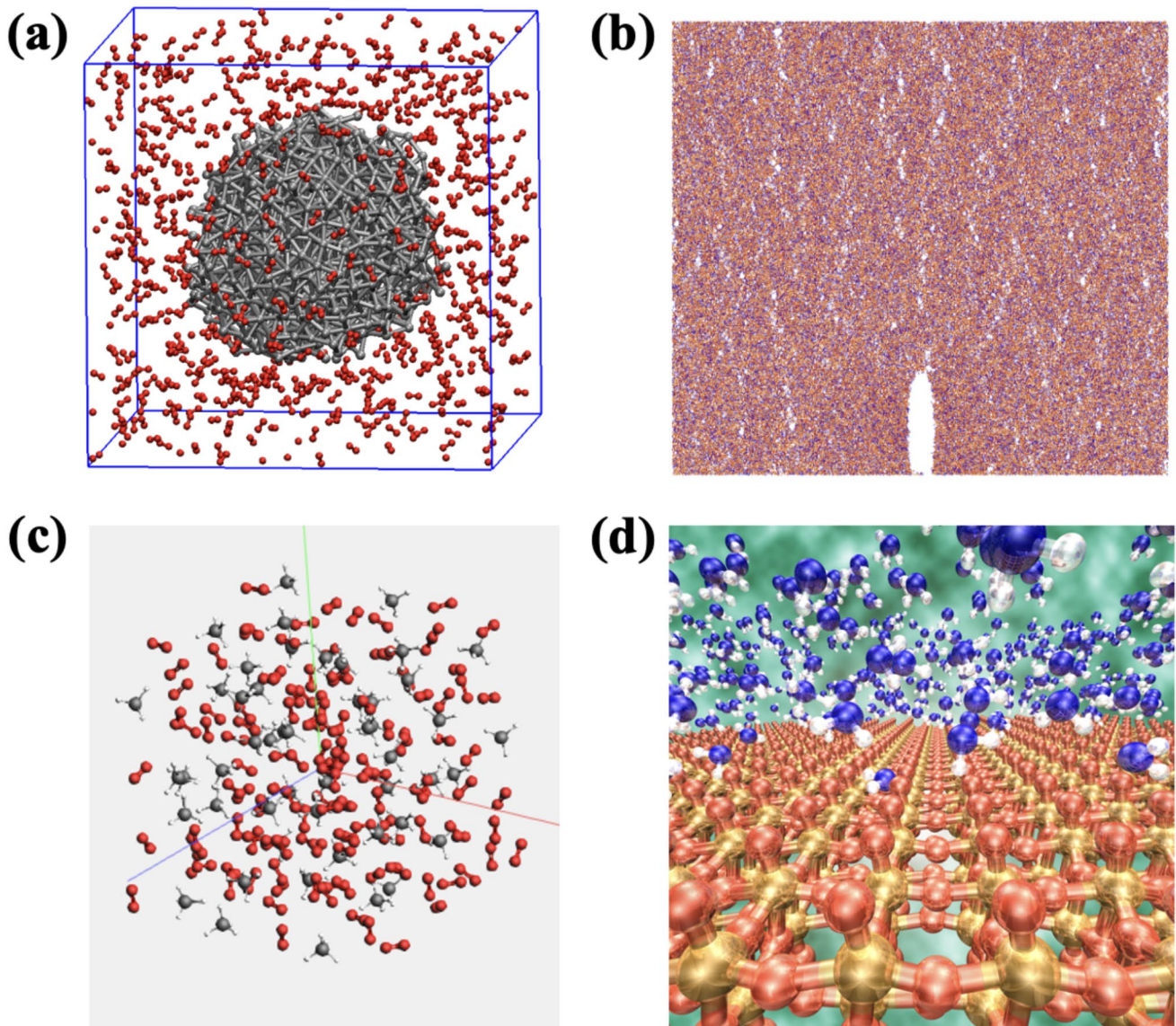


Fig. 1 Topics in computational materials science research integrated in our teaching module: **a** the oxidation of aluminum nanoparticle [14]; **b** fracture of glass–ceramics model [15]; **c** the oxidation of hydrocarbon fuel [16]; and **d** computational synthesis of semiconductor materials [17]

In conjunction with the pedagogical components, we implemented ReaxFF [22] based RMD simulation training—one of the in-demand skills in engineering—to enhance students’ foundational engineering knowledge and in learning. The RMD method utilizes computers to study a complex system of natural phenomena, allowing scientists to gain atomic-level insight into engineering problems involving chemically reactive processes, such as fuel oxidation and crack initiation in materials. This method is widely recognized as an effective tool for scientific discovery, as it provides insights and results that are often impractical to obtain through laboratory experiments or theoretical analysis. Furthermore, RMD increases efficiency in the problem-solving process by enabling iterative simulated experiments

and significantly reducing the costs associated with laboratory experiments. [23–25] Most importantly, RMD allows scientists to virtually manipulate key variables to explain phenomena, gain scientific insights, and make discoveries by providing atomic-level data on reactive processes. These processes can be visualized using external software such as VESTA, Jmol, XCrySDen, or Ovito.[26–29].

Participants and setting

We recruited participants from two Hispanic-serving institutions located in rural areas of central California—one regional four-year public university and one community college—through faculty recommendation, campus

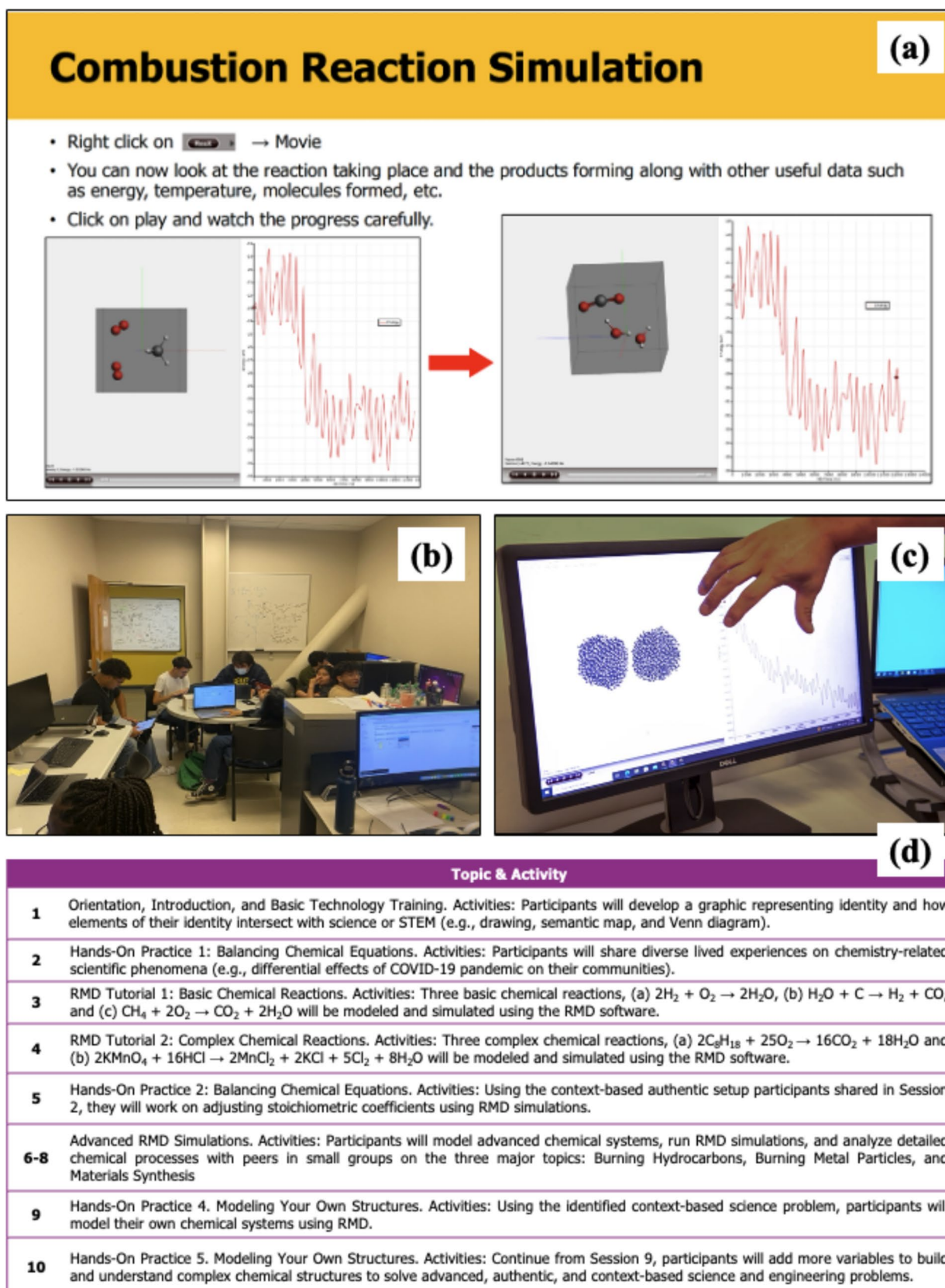


Fig. 2 **a** Example of step-by-step RMD modules developed for the oxidation of hydrocarbons; **b** snapshot of students participating in RMD training; **c** snapshot of the instructor providing hands-on instruction for RMD simulations; and **d** topics and activities of the program

advertisement, and email invitations. Students who completed the 10-session program received a stipend and a certificate of completion. Both institutions share similar characteristics in terms of the student body they serve, with 50–62.3% of students being female and 60–70% being Hispanic. A total of six students ($n = 6$), all in their first year of college in STEM majors, participated in the program. All participants were first-generation college students pursuing a baccalaureate or associate degree and came from low-income backgrounds. See Table 1 for participant demographic information.

Research design

A qualitative case study design was used to understand the complex interplay between students’ STEM identity and motivation among college students participating in a pilot study within a university research program. [30] This approach enabled us to explore both measurable changes in STEM identity and motivation, as well as student perceptions and personal experiences that quantitative data alone may not fully capture. This design provided insights into how a single program intervention could influence student outcomes, informing potential refinements for future implementations. [31] Prior to the study, we obtained approval from the Institutional Review Board to ensure that all procedures followed by ethical guidelines for research involving human participants. All participants provided informed consent before participating.

Conceptual framework

Among various conceptualizations of STEM identity, we adopted the latest STEM identity framework proposed by Hazari et al. [32] that expanded Carlone and Johnson’s [33] work. In Hazari et al.’s [32] framework, there are four inter-related dimensions of science identity: one’s own feelings or belief about (a) *performances* (i.e., feeling confident in their ability to perform their scientific practices and skills to others), (b) *competence* (i.e., feeling confident that they are capable of acquiring the knowledge necessary to understand STEM/science content), (c) *recognition* as a science person (i.e., feeling confident that others recognize their competence and performance), and (d) *interest* (i.e., persisting desire to engage with certain content). In addition to Hazari’s framework, we used Glynn et al.’s [34] framework, which identifies five sub-components for conceptualizing science motivation: students’ conceptualization, intrinsic motivation, self-determination, self-efficacy, career motivation, and grade motivation toward science.

Data collection and analysis

The pilot study collected data from two administered surveys, one focusing on identity as a STEM professional and the other on motivation to learn science, conducted at both the beginning and end of the program. Survey-based measures were chosen to quantify changes in STEM identity and motivation efficiently, while open-ended responses provided qualitative insights. We used the STEM Professional Identity Overlap (STEM-PIO-1) [35] measure, a single-item tool where participants were instructed to select the image that best describes the overlap between their self-image and their

Table 1 Participant demographics and descriptive data on STEM identity and science motivation

Name	Demographics				STEM Identity			Motivation Type				
	Gender	Ethnicity	Major	School	Before	After	% Diff	% Mean Diff				
	IT	CR	SD	SE	GR							
Amy	F	White	Physics	CC	33.33% (2)	100% (6)	66.67%	0	5	15	10	5
Eva	F	Hispanic	Pre-health	RPU	50.00% (3)	100% (6)	50.00%	25	10	20	30	10
Miguel	M	Hispanic	Electrical engineering	RPU	50.00% (3)	100% (6)	50.00%	10	20	5	15	0
Erik	M	Hispanic	Aerospace engineering	CC	33.33% (2)	83.33% (5)	50.00%	15	30	15	30	5
Sammy	F	Asian	Mechanical engineering	CC	16.67% (1)	83.33% (5)	66.66%	0	10	10	20	10
Santiago	M	Black	Computer science	RPU	16.67% (1)	83.33% (5)	66.66%	0	30	35	5	– 5
Total Mean	–	–	–	–	33.33% (2)	91.67% (5.5)	58.34%	8.33	17.5	11.67	18.33	4.17
Paired T-test	–	–	–	–	–	–	–	1.98	3.95	3.26*	4.35**	1.75

All names are pseudonyms

F female; M male; CC community college; RPU regional public university; Diff Difference; % Mean Diff indicates the difference between pre- and post-test scores; IT intrinsic; CR career; SD self-determination; SE self-efficacy; GR grade

Numbers in parentheses indicate scores on the original scale. * $p < 0.05$; ** $p < 0.01$

perception of what a STEM or science professional is. The measure uses a 7-point pictorial response scale to quantitatively assess students' perceived overlap with their desired future identity. Additionally, we used the Science Motivation Questionnaire II [34] to measure students' overall motivation to learn science. The questionnaire contains 25 items on a 5-point Likert scale (0: never to 4: always), with the highest possible score indicating high science motivation.

Data analysis followed a five-step thematic analysis process—organizing, sorting, understanding, interpreting, and explaining the data [36]—with the aid of computer-assisted qualitative data analysis software NVivo version 14. Open-ended responses were analyzed using thematic coding, employing a deductive approach based on Hazari et al.'s STEM identity framework, with pre-determined themes guiding the analysis. We sorted the data to create a coding structure, developed from the conceptual framework, which served as the basis for pre-determined codes used in deductive coding. [37] We interpreted the data using pattern coding, where the initial codes were clustered into patterns or themes. This process involved relating the study findings to the conceptual frameworks and relevant literature to assess how the study contributes to existing knowledge on STEM identity and science motivation. The explanation of the interpreted data is provided within the findings and discussion.

Result and discussion

All participants' self-perception of their STEM identity increased before and after participating in the program, as shown in Table 1 and Fig. 3. Similarly, as indicated in Table 1, all participants' self-perception of science motivation generally increased before and after the program, except for one participant, Sammy, whose science motivation score remained the same. A paired t-test was conducted to compare the pre- and post-program science motivation scores, which were measured using a Likert-scale survey. The analysis revealed that overall motivation significantly increased ($t = 6.10, p = 0.001$). Please refer to Table 1, where we present the differences in motivation across five subtypes after the program. This quantitative increase in motivation provides context for the qualitative themes that emerged. The following five components summarize the qualitative findings, which align with the statistical trend of increased motivation.

STEM identity: performance

Three of the six participants reported improved performance after completing the program, with two key themes emerging. First, enhanced learning skills. Participants highlighted

in both STEM-specific skills and general academic and learning skills, particularly teamwork. Eva reported increased confidence in peer collaboration. Miguel noted that group discussions and projects boosted his confidence, motivation, and overall attitude, stating, "*This program helped me with my confidence, motivation, and general attitude because of the group projects and discussions we would do to socialize more with one another.*" Sammy specifically credited the program's simulations for improving visualization and analytical thinking, explaining, "*I was critically able to analyze when coming across an error in my simulation and was able to fix the given error.*" Second, belief in one's ability to excel in STEM fields. Participants reported increased self-confidence and motivation as they progressed through the program. Miguel observed a steady improvement in his performance, which reinforced his belief in his abilities: "*After noticing I was doing well on the assignments, my confidence and motivation were high.*" He also emphasized that overcoming challenges during the program strengthened his determination to succeed in STEM.

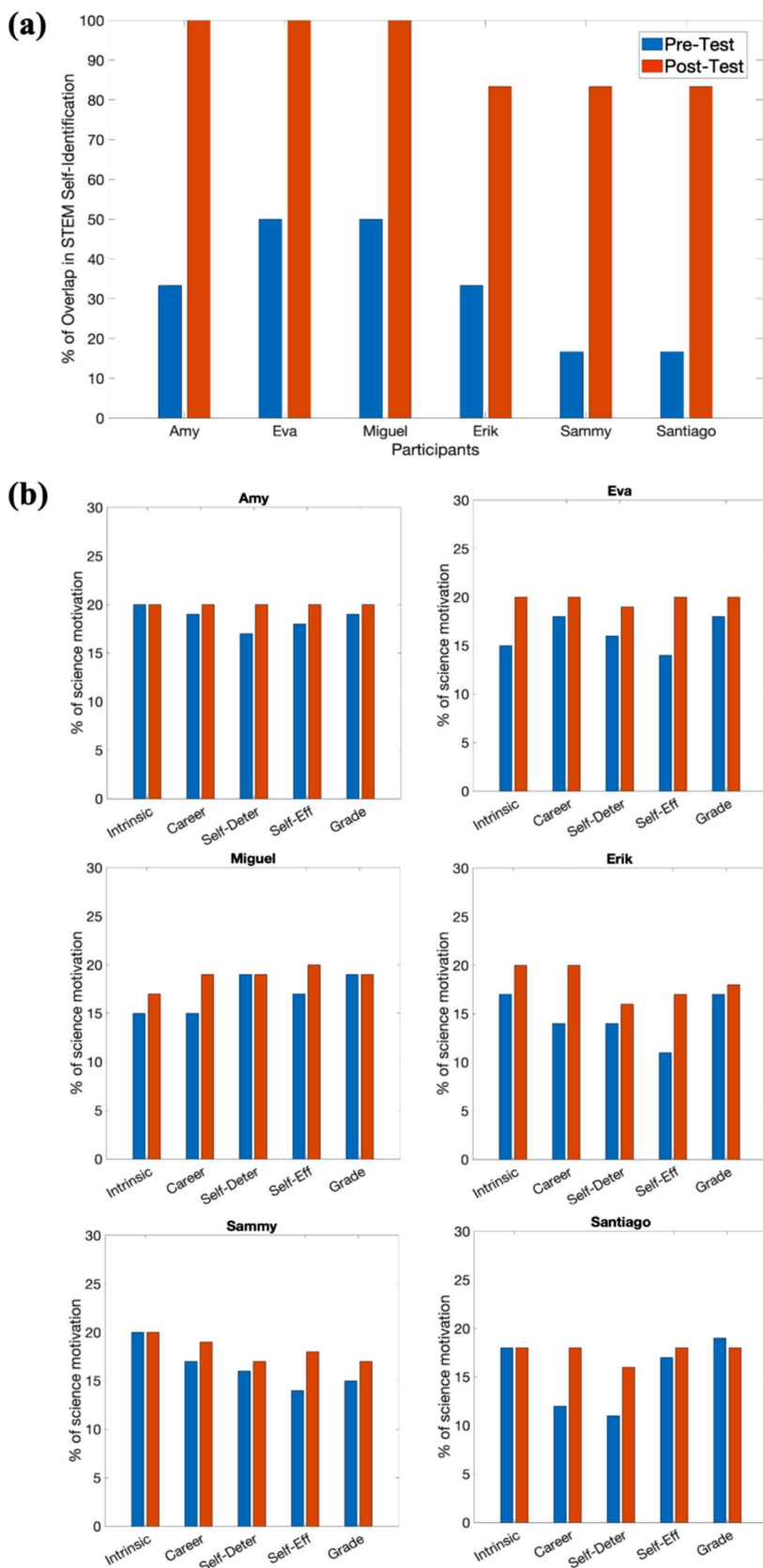
STEM identity: competence

Five of the six participants reported increased competence in STEM after completing the program, with a central theme emerging: a belief in gaining STEM knowledge. Participants described how the program deepened their understanding of STEM concepts. Miguel highlighted learning advanced insights through RMD: "*The techniques helped me take a deeper look at cracks in certain elements and oxidation.*" Erik emphasized bridging theoretical knowledge with practical applications, stating, "*This practical exposure allows me to bridge the gap between theoretical knowledge from engineering classes and real-world applications at the atomic scale.*" Santiago noted the complexity of college-level STEM compared to high school, saying, "*It brought to my attention the difference in volume and complexity.*" Eva valued the simulations for enhancing her understanding of chemistry and modeling techniques, while Sammy appreciated the program's fresh perspectives: "*Everything about this program was insightful and a new learning curve for me.*" Overall, participants highlighted the program's role in broadening their foundational and advanced STEM knowledge, with Erik adding, "*This tool is advantageous for fundamental chemistry concepts and understanding atomic structures.*"

STEM identity: recognition

All six participants reported an increased perception of STEM as part of their identity after the program. Five participants highlighted feeling ready to enter the STEM workforce. Amy noted, "*This program expanded my knowledge*

Fig. 3 a Changes in students' self-reported STEM identity, measured by the percentage of overlap in STEM self-identification; and **b** Changes in students' self-reported science motivation, comparing pre- and post-program responses



of engineering science from an academic perspective to a workplace perspective. I feel more prepared to enter a related workforce.” Erik and Miguel emphasized gaining transferable skills for their STEM fields. Two participants recognized the program’s simulation as a valuable introduction to workplace technology. Sammy stated, “*Learning computation simulation and modeling is an excellent skill and a great starting point in the world of software.*” Santiago recommended integrating similar simulations into all engineering classes, citing its relevance to real-world applications.

STEM identity: interest

Two participants reported increased interest in STEM fields after completing the program, expressing greater curiosity and a stronger commitment to pursuing STEM careers. The theme of engrossment in STEM fields emerged, reflecting participants’ curiosity and desire to deepen their STEM knowledge. Eva described newfound inquisitiveness about chemical reactions: “*I loved looking at the models... I’d like to discover more elements to see their reactions.*” Erik shared a similar desire to explore advancements in STEM: “*This experience has fueled my desire to delve deeper into engineering, conducting research, and contributing to improvements in the field.*” Both participants also expressed career-focused interest. Erik noted increased motivation to pursue engineering, while Eva highlighted the program’s role in sparking interest in a related field: “*This program helped me gain more knowledge in chemistry and discover more about engineering, which can benefit my future.*”

Motivation

The theme of motivating learning experiences emerged as five of six participants shared how the program inspired them to persevere in STEM fields. Key motivators that served as themes included the curriculum, collaborative work, and personal characteristics. For the curriculum, participants highlighted the simulation’s user-friendly design, opportunities to explore, and hands-on activities as motivating factors. Erik described the simulation as “*versatile and accessible.*” Amy expressed excitement about exploring its features: “*I was excited to learn how it worked in practice and what the settings could do.*” For the collaborative work, two participants found peer collaboration motivating. Miguel valued social support, while Amy appreciated lasting peer connections. For personal characteristics, Eva found enjoyment in the program’s activities: “*I had a lot of fun learning the different computational simulations.*” They also credited the program with motivating them to complete their education and pursue a STEM career.

Conclusion

The pilot study demonstrated positive indication that participation in the winter research program involving RMD had a beneficial impact on students’ perceptions of their STEM identity and motivation. Six participants provided responses through a survey that included both close-ended and open-ended questions, with responses analyzed using a STEM identity and motivation framework. Key findings are the following. First, participants reported improvements in interest, competence, performance, and recognition within STEM fields. They became more engaged in STEM through curiosity-driven exploration, enhanced their STEM skills and knowledge, and gained confidence in their ability to succeed in STEM-related fields. Second, the program motivated participants to persist in STEM learning. Positive learning experiences, such as engaging in hands-on activities, peer collaboration, and the use of simulations, were significant motivators despite some challenges during group work. Overall, the program demonstrated promise in fostering students’ STEM identity and motivation, promoting both personal and academic growth in STEM fields. These findings have educational implications for integrating RMD. However, further validation is needed to strengthen these conclusions based on the preliminary results.

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Author contributions J. L. H., S. L. H., and J. S. designed, implemented, and supervised the study; T. M. analyzed the qualitative data; J. H. conducted a literature review; and P. L. and K. F. conducted RMD simulations and developed and refined RMD modules. All the authors contributed to the current study.

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Data availability The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

Conflict of interest The authors declare that there is no conflict of interest to declare.

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