CHEMICALEDUCATION

Baltimore SCIART: A Fully Virtual Undergraduate Research Experience at the Interface of Computational Chemistry and Art

Jessica E. Heimann, Tory H. Williams, Joseph W. Bennett, and Zeev Rosenzweig*



ABSTRACT: From its inception in 2016 through 2019, the Baltimore SCIART Consortium offered an annual 10-week interdisciplinary summer research program for undergraduate students. Each year, the program mentored approximately 10 students, many from primarily undergraduate institutions including minority serving institutions and historically black colleges and universities. Throughout the sessions, the students were exposed to the career paths of art conservation and art conservation science as they worked in the laboratories of scientists, engineers, art conservators, and art conservation scientists at the University of Maryland Baltimore County, Johns Hopkins University, and the Walters Art Museum in Baltimore. Preparations for the 2020 program were underway when the COVID-19 pandemic shifted the undergraduate research paradigm to a virtual experience. An inperson, laboratory-based program was no longer an option, and this challenged the SCIART team to investigate novel ways to offer a rigorous, engaging undergraduate research program in a fully virtual setting. The result was an intensive, three-week pilot program in which four SCIART students learned about and successfully applied open-source periodic density functional theory software packages to explore the interactions between small molecule adsorbates and mineral-based surfaces relevant to art conservation. This case study exemplifies how educators and research leaders were able to strategically pivot and provide an adapted curriculum for a unique, interdisciplinary, and fully virtual undergraduate research experience. The implication is a potential (scalable) model for culturally engaging research opportunities for historically underrepresented students in STEM, both during and beyond the COVID-19 pandemic.

KEYWORDS: Second-Year Undergraduate, Upper-Division Undergraduate, Curriculum, Inorganic Chemistry, Physical Chemistry, Computational Chemistry, Interdisciplinary/Multidisciplinary, Collaborative/Cooperative Learning, Computer-Based Learning

■ INTRODUCTION

The Baltimore SCIART Consortium¹ began in 2016 as an annual 10-week summer research experience for undergraduate students at the interface of science and art (SCIART). Students selected for this program included those majoring in chemistry, biology, engineering, visual arts, and history; many came from primarily undergraduate institutions (PUIs) and historically black colleges and universities (HBCUs). Each year, the program enrolled approximately 10 students to conduct research in the laboratories of scientists, engineers, and art conservators at the University of Maryland Baltimore County (UMBC), Johns Hopkins University (JHU), and the Walters Art Museum (WAM) in Baltimore. For the first four years of SCIART, the primary goal of the interdisciplinary under-

graduate research experience was to combine hands-on, laboratory-based scientific training with exposure to the fields of art conservation and art conservation science. The students also participated in professional development activities and built connections with practicing art conservators/conservation scientists. Preparations for a similar program in the summer of

Received: April 13, 2021 Revised: June 5, 2021 Published: September 2, 2021





Journal of Chemical Education

2020 were underway when the COVID-19 pandemic shifted both the education and undergraduate research paradigm to primarily virtual experiences. The original 2020 program was canceled since an in-person program was no longer an option, but this unprecedented challenge prompted the question of whether a fully virtual undergraduate research experience that combines hands-on, *computational* scientific training with exposure to the fields of art conservation and art conservation science was possible. Further, might the same caliber of professional development be integrated into a fully virtual research program? The SCIART program was reimagined and implemented as a three-week, fully virtual research program during the winter semester of 2021, and the outcomes of the pilot program suggest a successful, rigorous experience for students.

The importance of offering undergraduate research programs that focus on computational chemistry is 2-fold. First, computational methods such as those based on density functional theory (DFT) or molecular mechanics remain underutilized tools in the undergraduate chemistry curriculum. Although there have been several examples of successfully integrating computational methods into the undergraduate lecture or laboratory curriculum throughout the past 15 years,²⁻¹³ nearly all examples involve isolated molecules that employ an atom-centered basis set, and many require the purchase of licensed software packages. This excludes students in smaller undergraduate programs or programs that lack a heavy focus on science, technology, engineering, and mathematics (STEM), where the high cost of these software packages may be prohibitive. Moreover, most undergraduate students are not exposed to computational methodologies used to explore bulk materials and surface phenomena of materials common to art conservation and cultural heritage including copper, lead alloys, and minerals. Specifically, surface adsorption calculations analyzing the interactions between common atmospheric pollutants and a material surface can provide valuable insight into the physiochemical and surface properties of the material. Understanding these interactions plays a critical role in the development of noninterventive methods to assess and protect cultural heritage artifacts. This type of computation employs plane wave basis sets, which are primarily applied in solid-state physics research and less commonly in computational chemistry. As a result, chemistry students may lack essential knowledge about solid-state surface calculations that could augment their understanding of both class-based and independent research. Given the rapidly increasing use of computational methods in almost every application and subdivision of chemical research, it is imperative that the next generation of scientists can recognize, interpret, and perform simulations, a goal that aligns with one of the 10 Big Ideas of the National Science Foundation (NSF): harnessing the data revolution.¹⁴ Second, utilizing a virtual platform for a hands-on program means that students who, for a multitude of reasons, cannot reside or travel to/from campus on a daily basis can still have an authentic, open-ended research experience at home. By including students who may lack transportation to/from campus or have family and/or work commitments, the SCIART program works to broaden participation in scientific research.¹⁵ The ongoing global COVID-19 pandemic has created the opportunity to initiate a remote approach to effectively teaching chemistry, and several recent publications have discussed how to best use online resources to effectively teach chemistry in a virtual setting.^{16–21}

There are, however, fewer reports about harnessing computational methods to virtually conduct chemical research.

In this article, we present a case study for implementing a unique interdisciplinary computational research experience for undergraduate students using a fully virtual platform. First, we provide the educational context and program goals, including both the general SCIART goals and the more specific computational aims. Next, we discuss the four phases of the program including topics and exercises covered within each phase. Last, we provide specific details on how the SCIART program utilizes DFT (a quantum mechanical method used to calculate the electron density of atoms, molecules, and condensed matter) to gain insight about a system of interest. Overall, the recent Baltimore SCIART program provides a promising example of the successful adaptation of the undergraduate research curriculum in response to an unprecedented challenge. The program design and exercises adopted here can provide valuable insight for other instructors, research programs, and institutions, particularly those that wish to incorporate virtual learning into their core curriculum. The outcomes of this work will bring continued value to virtual learning that extends into the future of higher education.

EDUCATIONAL CONTEXT AND PROGRAM GOALS

The Baltimore SCIART Consortium was established as a collaboration between UMBC, JHU, and Morgan State University (MSU) with the WAM to provide interested undergraduate students with a platform to investigate the underexplored interface between science and art. Since its inception, the SCIART program has exposed approximately 40 undergraduate students to cutting-edge research in the laboratories of scientists, engineers, and art conservators and conservation scientists at the three participating institutions. The program is designed for high-performing undergraduate students with diverse interdisciplinary interests, specifically (1) science or engineering students with a strong interest in art and art conservation/conservation science or (2) humanities students with science or engineering backgrounds. Completion of introductory level chemistry lecture and laboratory courses prior to the program is mandatory for all participants, while courses such as organic, inorganic, and physical chemistry are recommended (but not required).

The primary goal of the SCIART program is to combine hands-on scientific training with exposure to the fields of art conservation and art conservation science. A significant component of this is providing students with the opportunity to directly connect and interact with practicing art conservators and conservation scientists at museums such as the WAM in Baltimore, the Metropolitan Museum of Art in New York City, and the National Gallery of Art in Washington, DC. Furthermore, the program also incorporates mandatory professional development activities that ensure that each student, regardless of their chosen career path, learns skills to advance along that path. For example, the 2019 SCIART program included the following two 2 h professional workshops: (1) Presentation Skills: How to Make a Good Oral and/or Poster Presentation and (2) Presenting Your Research: Effective Scientific Posters. In addition to the goals outlined above, the three-week computational SCIART program in January 2021 also sought to:

 Teach the students to use common Linux commands to access and submit jobs to a facility for scientific computing

Та	b	le	1.	Ph	ases	of	Com	putat	tional	SCIA	RТ	Research	Program
----	---	----	----	----	------	----	-----	-------	--------	------	----	----------	---------

Phase	Pedagogical Approach and Focus	Exercises for Students
1	Preprogram training sessions	Participate in demonstrations of computing concepts and terms
		Learn definitions and view examples of common Linux commands
		Attend an introductory DFT lecture
2	(Week 1) Structured lectures and guided exercises	Generate bulk structure of aragonite from standardized crystal structure data (Figure 1)
		Relax structure with periodic DFT
		Create and relax supercell surface slab (Figure 2)
		Study adsorption of four similar small molecules on calcium-terminated surface (Figure 3)
3	(Week 2) Independent exploration	Search through relevant literature to identify additional adsorbates
		Expand list of small molecules and atmospheric pollutants to include student-chosen adsorbates
		Generate charge density and charge density difference plots for selected surface adsorption calculations (Figure 4)
4	(Week 3) Data interpretation and scientific communication	Analyze full body of data to draw conclusions and interpret results in context of art conservation
		Work as a team to design and create a presentation and poster summarizing the project
		Present work to an audience of undergraduate and graduate students, professors, and art conservators and conservation scientists

- (2) Introduce the students to the general principles of DFT
- (3) Demonstrate how to use open-source plane wave-based DFT packages to study the interactions between small molecule adsorbates and mineral-based surfaces relevant to works of art
- (4) Create a space for the students to explore how the combination of experimental and computational data is more compelling than either in isolation and, thus, present a more rigorous approach to research
- (5) Provide an inquiry-based, impactful research experience to students using a fully virtual (at home) platform

Although introductory materials for plane wave-based computational methodologies exist,^{22,23} we find that there is a serious disconnect between the level of knowledge needed to understand these tutorials/workshops and the level of knowledge undergraduate students have on the relevant subjects. The materials available, which are primarily online tutorials, are aimed at teaching advanced STEM undergraduate and early graduate students how to run and interpret DFT calculations. These tutorials presuppose a working knowledge of Fortran, quantum mechanics, inorganic chemistry, and differential equations that are beyond the curriculum of many of the students selected to participate in the SCIART program. The recent computational SCIART program aimed to bridge this gap and provide the students with the information needed to access and understand the available resources, both during and after the program. An important tool in achieving these goals is the High Performance Computing Facility (HPCF),²⁴ an interdisciplinary, community-based core facility for scientific computing and research at UMBC. Provided with an account at the UMBC HPCF for the duration of the program, each SCIART student was able to access the computing cluster (with over 90 CPU nodes connected by a high-performance network communication system²⁵) to submit, run, and interpret their calculations. Specifically, the students were provided access to an opensource DFT software package called Quantum ESPRESSO. Quantum ESPRESSO^{26,27} is a suite of open-source computer codes that allows scientists to use DFT to perform electronicstructure calculations and model materials. Specific descriptions and examples of the calculations performed in the SCIART program are discussed below, and additional resources including example input files and a Quantum ESPRESSO runscript are provided in the Supporting Information. While UMBC has

access to high-performance computing facilities, we recognize that some institutions or instructors that may be interested in organizing similar research experiences do not. Programs of this type may benefit from an NSF-XSEDE Education Allocation.²⁸ The NSF-XSEDE program allots up to 50,000 h of runtime for specific classes and courses, in which students can log on and run simulations on some of the most powerful supercomputers in the United States.

PROGRAM DESIGN AND DISCUSSION

To achieve the goals outlined above, the recent SCIART program was designed to include four phases (Table 1), each with its own focus and instruction type. The following paragraphs describe the phases sequentially and provide an indepth discussion on each phase, highlighting how the content of the program advanced throughout the four phases. It should also be noted that the participants were provided with laptops for the duration of the program, and each laptop had all the necessary software installed prior to student pick-up. All open-source software used throughout the SCIART program is listed in the Computational Methods and Resources section below.

Phase 1: Preprogram Training Sessions

The first phase of the computational SCIART program focused on introducing the students to computing and the basics of DFT, as the students did not have any experience with either prior to this experience. Phase 1 occurred before the program start date as three 2–3 h training sessions. One session was an introductory DFT lecture and discussion (the contents of which are described in the Supporting Information), and the other two primarily consisted of guided demonstrations in which the students actively participated and performed the exercises on their laptops. To ensure that the students did not fall behind, questions were encouraged, and each student was asked to share their screen at multiple points throughout the sessions. The computing topics included in the two training sessions were as follows:

- (1) Accessing and logging onto the UMBC HPCF cluster
- (2) Creating and navigating the directory system
- (3) Copying and untarring (unzipping) files
- (4) Editing pre-existing files to create new input files
- (5) Submitting jobs to the cluster using a queue management software known as a SLURM queue

Journal of Chemical Education

Article

- (6) Reading the output file
- (7) Transferring files from the cluster to their local computer
- (8) Visualizing structures and charge density

As evident in the list above, these training sessions were not chemistry focused. The goal was to familiarize the students with computing concepts that they would be exposed to during the program.

Phase 2: Structured Lectures and Guided Exercises

The focus shifted to chemistry between phase 1 and 2, as the students were required to read the provided background literature on aragonite (a polymorph of calcium carbonate and the chosen mineral for our study) and fundamental (as well as accessible) DFT articles.^{29–32} Aragonite was selected for the SCIART project for two reasons. First, the mineral has a strong connection to cultural heritage and art conservation as a component of (1) historical pigments and paints, (2) materials such as limestone and marble, and (3) the shells of mollusks.³³ Second, the chemical formula of aragonite (CaCO₃) does not include a transition metal (i.e., redox) or heavy metal (i.e., spin–orbit coupling), which significantly reduces the computing time and power required to fully relax surface structures. Reasonable computing times were crucial, as the program was only 3 weeks in length.

Phase 2 was the first week of the program and incorporated daily structured lectures and guided exercises and frequently reapplied the terms introduced during the preprogram training sessions (phase 1) to reinforce those concepts. There were three primary objectives for phase 2: (1) guide the students through the process of computationally generating the bulk structure from standardized crystal structure data, (2) demonstrate how to create the supercell surface slab from the relaxed bulk structure, and (3) aid the students in setting up the first round of surface adsorption calculations. As the main goal of the student research project was to study the physiochemical and surface properties of aragonite by exploring the interactions between common small molecule pollutants and the mineral surface, the first two primary objects in phase 1 were essential in creating an accurate (i.e., based on experimental data) computational model of the chosen material. To obtain the necessary standardized diffraction data, the first objective included a tour of available crystal databases and online tools such as The Materials Project³⁴ that do not require a subscription or fee to search (see Supporting Information for specific modules explored). The bulk structure generated from the experimental crystal data (Figure 1) also served as the starting point in a lecture about crystal systems and symmetry elements in extended solids. In a visual demonstration of translating the primitive unit cell in three dimensions, cleaving along a specific crystallographic axis, and then introducing vacuum to create an inversion symmetric, calcium-terminated supercell surface structure (Figure 2), the students then addressed the second objective.

In phase 2, the students were also guided through the process of setting up their first surface adsorption calculation by adding a small molecule adsorbate to the supercell surface slab. They started with four very similar adsorbates (CO_2 , NO_2 , SO_2 , and O_3), which prompted a discussion on functional groups and how different, more complex functional groups could interact with the calcium-terminated aragonite surface. With the incorporation of physical models of the functional groups of interest, this discussion proved particularly valuable for nonchemistry majors and the students who were less familiar with the structures and binding motifs of common functional groups. A representative



Figure 1. Bulk structure of aragonite. Calcium, carbon, and oxygen are shown in teal, gray, and red, respectively. The primitive unit cell is outlined in green.



Figure 2. Supercell surface slab of aragonite generated from relaxed bulk structure. Symmetry elements are shown in black.

surface adsorption structure is provided in Figure 3. As a followup question to modifying the functional group on the adsorbate, the students were also asked to hypothesize about the effects of changing the aragonite surface termination. Specifically, they were shown a model of a protonated aragonite surface slab in which the two surface calcium atoms had been removed and protons subsequently had been added to balance the charge. This model is in line with those used in similar surface exchange calculations.^{35–38} Exploring this protonated structure introduced the students to the concept of DFT + thermodynamics calculations,^{39–41} which were the focus of our final internal



Figure 3. Sulfur dioxide (SO_2) physisorbed on the aragonite surface. Sulfur is shown in yellow.

seminar during the three-week program (see Supporting Information for additional information). Running the surface adsorption calculation with CO_2 , NO_2 , SO_2 , or O_3 was also the first time that each student had an individual goal. The SCIART project was designed to have a balance of both team-based and individual elements.^{42,43} With the individual elements, we aimed to provide enough similarity between them that the students could help and use one another as resources if needed, but we also wanted each student to feel ownership and individual responsibility over one or more specific aspects of the project.

Phase 3: Independent Exploration

During the second week of the program (phase 3), the pedagogical approach progressed from structured lectures and guided exercises to independent exploration. The first objective for phase 3 was to expand the list of small molecules and atmospheric pollutants to investigate in the study. To do so, the students were asked to search the art conservation/art conservation science literature and identify small molecules and pollutants that have been experimentally shown to negatively impact an aragonite surface or artifact in some way. From the literature collected by the students, ^{44–48} the following adsorbates were chosen (in addition to CO_2 , NO_2 , SO_2 , and O_3 , which were studied in phase 2):

- (1) H_2O
- (2) H_2S
- (3) SO_3
- (4) H_2SO_3
- $(5) H_2 SO_4$
- $(6) CH_2O$
- (7) HCOOH
- (8) CH₃COOH

This group of 12 adsorbates included different molecule types and functional groups, which allowed the students to make comparisons across variables such as (1) 2p vs 3p valence shell, (2) carbon- vs nitrogen- vs sulfur-centered, and (3) linear vs bent vs tetrahedral geometry around the central atom. Further discussion on the analysis and interpretation of the data is included in the description of phase 4 below. The independent literature search was also used as an opportunity to emphasize

pubs.acs.org/jchemeduc

that computational methodologies represent an extremely underutilized tool in art conservation and art conservation science. The dearth of available literature in which computational chemistry is applied to an art conservation question highlighted a mostly unexplored avenue of research, and this observation motivated a discussion about the value of computational studies and the power of combining experimental and computational data to more thoroughly answer the question at hand. This idea was then extended, and the students were asked to consider the limitations of a purely computational approach, mainly that our model represents a perfect (defectless) system at zero temperature and pressure. Guided by specific questions from the instructor, the students arrived at the conclusion that the information obtained from this type of calculation is still valuable to art conservators, as it identifies general trends in surface reactivity that can then be interpreted in their work or probed experimentally.

The second objective in phase 3 was to visualize the charge density in selected calculations and explore the type of information we can extract from a charge density difference plot, which is a comparison of where the electron density lies when the adsorbate is and is not present. A representative charge density difference plot is provided in Figure 4, and additional



Figure 4. Charge density difference plot of sulfur dioxide (SO_2) physisorbed on the aragonite surface. The yellow color represents positive charge density (i.e., more charge density when the adsorbate is present), and the aqua blue color represents negative charge density (i.e., more charge density when the adsorbate is not present). For clarity, the charge density on the adsorbate has been subtracted from the figure.

information about postprocessing tools is provided in the Supporting Information. This type of visualization is a powerful qualitative tool, as it allows the students to see how the electron density on the surface is perturbed in response to an adsorbate, which again proved particularly valuable for the nonchemists and visual learners in the group.

Phase 4: Data Interpretation and Scientific Communication

As the first objective in phase 4, the students analyzed the full body of data qualitatively (by visualizing the perturbations in charge density, as described above) and quantitatively (by calculating the adsorption energy for each adsorbate; see <u>Supporting Information</u> for calculated values). On the basis of their observations, the students were first asked to draw conclusions on a purely scientific basis. Example discussion questions are provided below:

(1) Do the carbon-, nitrogen-, or sulfur-centered molecules interact with the aragonite surface most strongly?

pubs.acs.org/jchemeduc

- (2) How does adsorption energy (i.e., the strength of the interaction) correlate with pK_a for this series of adsorbates?
- (3) Describe the orientations of the acids on the aragonite surface. Do all adsorbates with a carboxylic acid functional group interact in the same orientation? How does the carboxylic acid orientation compare to that of an aldehyde?

Following this discussion, the students were then directed to frame their results/conclusions within the field of art conservation by asking the question "What preservation or conservation measures would you suggest to a conservator based on your findings?" An example response might be "A conservator preserving an aragonite artifact should focus on removing sulfurous gases from the storage or display environment, as these atmospheric pollutants were found to adsorb to the surface most strongly." This conversation was also a good opportunity for the students to hypothesize (based on the data they collected as well as previous studies⁴⁹) what would happen in more complex systems (i.e., with multiple interacting adsorbates present), as these scenarios are more representative of the chemistry occurring on the surface of a work of art or cultural heritage object.

Articulating their responses to the above questions along with designing and creating a presentation and poster to summarize the project also led the students to focus on communication and presentation skills in phase 4 (the second objective during the last week of the program). Teamwork was also a key skill developed during this week, as the students had to pull from their unique backgrounds and strengths to create a single cohesive, concise presentation. At the SCIART Showcase on the final day of the program, the students shared that presentation with an audience of undergraduate and graduate students, professors, and art conservators and art conservation scientists. This showcase was a celebration of what the students had accomplished during the program as well as another opportunity for the students to engage with practicing art conservators and art conservation scientists. The students were, thus, exposed to an authentic forum for communicating their scientific findings to experts in related fields, a paramount step in the scientific process.

COMPUTATIONAL METHODS AND RESOURCES

All calculations performed by students in the SCIART program employed periodic DFT methods^{29,30} using Quantum Espresso, an open-source software package.^{26,27} The atoms were represented using the open-source GBRV-type ultrasoft pseudopotentials,^{50,51} and a plane wave cutoff of 40 Ry and charge density cutoff of 320 Ry were employed for all calculations. Bulk structural relaxations used a $6 \times 6 \times 6$ kpoint grid,⁵² and the convergence criterion for self-consistent relaxations was 5×10^{-6} eV. Geometry optimization of all surface-adsorbate interactions did not include fixing any layers;⁵³ all atoms were free to relax. All calculations were performed at the generalized gradient approximation (GGA) level using the Wu–Cohen (WC) modified PBE-GGA exchange correlational functional for solids.^{54,55} The structures and charge density difference plots generated by the calculations were analyzed using XCrySDen⁵⁶ (Figures 1, 2, and 3) and VESTA (Figure 4),⁵⁷ respectively. As all software used in this program is open source, there is no charge associated with installing and using the necessary software.

SUMMARY AND OUTLOOK

The recent SCIART program demonstrates the feasibility of offering an interdisciplinary undergraduate research experience using a fully virtual platform. In 3 weeks (plus three 2-3 h training sessions), four students were able to not only learn the basics of computing and using an open-source DFT software package, but also apply that knowledge to answering a real question posed by art conservators and art conservation scientists: How do atmospheric pollutants and other small molecule adsorbates interact with an aragonite surface? Each student, regardless of their background and area of study, could provide both quantitative (e.g., adsorption energies) and qualitative (e.g., charge density perturbations, molecular or functional group conformations) evidence to address this question by the end of the program. Although the SCIART program used periodic (plane wave-based) DFT as a tool within art conservation science, similar programs could be designed to extend this computational methodology to other applications. Furthermore, as all the software used in this program is open source and can be installed and used on local computers, the content structure described above (and, therefore, a similarly designed program) is potentially scalable, meaning a larger group of students could also be engaged. These open-source codes are also installed on multiple XSEDE resources that are available for institutions that do not have on-campus access to high-performance computing facilities.

As only four students participated in the recent program, a quantitative assessment of their feedback would not be reliable. However, the students were asked to complete reflections at the end of each program week, and qualitative analyses of these weekly reflections were performed in order to identify emergent themes in their experiences and help recognize areas of improvements for future iterations of the SCIART program. Two major themes emerged from these analyses: (1) the growth mindset of the instructors and (2) the growth mindset of the students. As the first research program of its kind, the SCIART instructors had to listen and act on participant feedback to ensure that the students were actively learning throughout the program. Specifically, pedagogical adjustments were made on a weekly basis (based on the feedback received in the reflections from the previous week) to create a productive and evolving learning environment, which the students praised in their evaluations. The growth mindset of the students, on the other hand, was perhaps most evident in their self-reported comfort level in discussing weekly concepts and terminology. A detailed explanation of the qualitative analysis methods used as well as a more in-depth discussion of the identified patterns is provided in the Supporting Information.

Overall, the program was well-received by the students, and the varied backgrounds, skill sets, and readiness levels of the four participants (who all appreciated and grew from the SCIART program) demonstrate how this unique, interdisciplinary approach can provide a rigorous and engaging research experience for a variety of students. The SCIART program represents a unique way to connect with undergraduate students from diverse backgrounds with little to no formal computational training and enhance their computational literacy. The program design and exercises outlined here serve as a starting point for educators interested in providing undergraduate research experiences using fully virtual platforms. Such experiences may prove crucial in not only addressing the limited amount of computational chemistry currently in the undergraduate curriculum, but also making research more accessible for students who cannot travel to and from campus for in-person research.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.1c00425.

(1) Presentation/lecture outlines, (2) example input files for four different types of calculations, (3) an example runscript for Quantum ESPRESSO, (4) an explanation of the postprocessing tools used in the program, (5) timing information for a representative calculation, (6) results of the adsorption studies on a calcium-terminated aragonite surface, and (7) qualitative analyses of the semistructured student feedback (PDF, DOCX)

AUTHOR INFORMATION

Corresponding Author

Zeev Rosenzweig – Department of Chemistry and Biochemistry, University of Maryland Baltimore County, Baltimore, Maryland 21250, United States of America; orcid.org/0000-0001-6098-3932; Email: zrosenzw@ umbc.edu

Authors

- Jessica E. Heimann Department of Chemistry and Biochemistry, University of Maryland Baltimore County, Baltimore, Maryland 21250, United States of America; orcid.org/0000-0002-1050-4582
- Tory H. Williams Center for the Advancement of Learning and Teaching, University of Maryland Baltimore County, Baltimore, Maryland 21250, United States of America; orcid.org/0000-0002-3600-1174
- Joseph W. Bennett Department of Chemistry and Biochemistry, University of Maryland Baltimore County, Baltimore, Maryland 21250, United States of America; orcid.org/0000-0002-7971-4772

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jchemed.1c00425

Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

The Baltimore SCIART Program is supported by the Andrew W. Mellon Foundation under award 41500634. Additional funding for the computational program was provided by the Extreme Science and Engineering Discovery Environment (XSEDE)²⁸ start-up grant TG-CHE190075 and renewal allocation TG-CHE200108, which are supported by National Science Foundation grant ACI-1548562. All calculations were performed using the UMBC High Performance Computing Facility (HPCF). The acquisition of equipment for the UMBC HPCF is partially supported by the National Science Foundation, whose support we gratefully acknowledge and which requires the following notice: This material is based upon work supported by the National Science Foundation under the MRI grants CNS-0821258, CNS-1228778, and OAC-1726023, and the SCREMS grant DMS-0821311. We would also like to thank our collaborators Glenn Gates and Julie Lauffenburger at

the Walters Art Museum, who helped us identify aragonite artifacts (such as mask stone carving from the Late Formative or Late Preclassic period shown in the Abstract graphic) in the WAM collection.

REFERENCES

(1) Baltimore SCIART. https://sciart.umbc.edu (accessed March 2021).

(2) Hessley, R. K. A Computational-Modeling Course for Undergraduate Students in Chemical Technology. J. Chem. Educ. 2004, 81 (8), 1140.

(3) Pearson, J. K. Introducing the Practical Aspects of Computational Chemistry to Undergraduate Chemistry Students. *J. Chem. Educ.* 2007, 84 (8), 1323.

(4) Rowley, C. N.; Woo, T. K.; Mosey, N. J. A Computational Experiment of the Endo versus Exo Preference in a Diels-Alder Reaction. J. Chem. Educ. 2009, 86 (2), 199.

(5) Clauss, A. D.; Nelsen, S. F. Integrating Computational Molecular Modeling into the Undergraduate Organic Chemistry Curriculum. *J. Chem. Educ.* **2009**, *86* (8), 955.

(6) McNaught, I. J. Testing and Extending VSEPR with WebMO and MOPAC or GAMESS. J. Chem. Educ. 2011, 88 (4), 421–425.

(7) Linenberger, K. J.; Cole, R. S.; Sarkar, S. Looking Beyond Lewis Structures: A General Chemistry Molecular Modeling Experiment Focusing on Physical Properties and Geometry. *J. Chem. Educ.* **2011**, *88* (7), 962–965.

(8) Johnson, L. E.; Engel, T. Integrating Computational Chemistry into the Physical Chemistry Curriculum. *J. Chem. Educ.* **2011**, *88* (5), 569–573.

(9) Clausen, T. P. Combining a Standard Fischer Esterification Experiment with Stereochemical and Molecular-Modeling Concepts. *J. Chem. Educ.* **2011**, 88 (7), 1007–1009.

(10) Simeon, T.; Aikens, C. M.; Tejerina, B.; Schatz, G. C. Northwestern University Initiative for Teaching NanoSciences (NUITNS): An Approach for Teaching Computational Chemistry to Engineering Undergraduate Students. *J. Chem. Educ.* **2011**, *88* (8), 1079–1084.

(11) Wang, L. Using Molecular Modeling in Teaching Group Theory Analysis of the Infrared Spectra of Organometallic Compounds. J. Chem. Educ. **2012**, 89 (3), 360–364.

(12) Hoffman, G. G. Using an Advanced Computational Laboratory Experiment To Extend and Deepen Physical Chemistry Students' Understanding of Atomic Structure. *J. Chem. Educ.* **2015**, *92* (6), 1076– 1080.

(13) Esselman, B. J.; Hill, N. J. Integration of Computational Chemistry into the Undergraduate Organic Chemistry Laboratory Curriculum. *J. Chem. Educ.* **2016**, 93 (5), 932–936.

(14) NSF's 10 Big Ideas: Harnessing the Data Revolution. https:// www.nsf.gov/news/special_reports/big_ideas/harnessing.jsp (accessed April 2021).

(15) Strategic Plan for the National Academy of Sciences: 2020–2025. http://www.nasonline.org/about-nas/nas-strategic-plan/2025-strategic-plan.pdf (accessed March 2021).

(16) Dukes, A. D., III Teaching an Instrumental Analysis Laboratory Course without Instruments During the COVID-19 Pandemic. *J. Chem. Educ.* **2020**, 97 (9), 2967–2970.

(17) Müssig, J.; Clark, A.; Hoermann, S.; Loporcaro, G.; Loporcaro, C.; Huber, T. Imparting Materials Science Knowledge in the Field of the Crystal Structure of Metals in Times of Online Teaching: A Novel Online Laboratory Teaching Concept with an Augmented Reality Application. J. Chem. Educ. **2020**, 97 (9), 2643–2650.

(18) Nyachwaya, J. M. Teaching General Chemistry (I) Online during COVID-19. Process, Outcomes, and Lessons Learned: A Reflection. *J. Chem. Educ.* **2020**, *97* (9), 2935–2939.

(19) Perets, E. A.; Chabeda, D.; Gong, A. Z.; Huang, X.; Fung, T. S.; Ng, K. Y.; Bathgate, M.; Yan, E. C. Y. Impact of the Emergency Transition to Remote Teaching on Student Engagement in a NonSTEM Undergraduate Chemistry Course in the Time of COVID-19. J. Chem. Educ. **2020**, 97 (9), 2439–2447.

(20) Villanueva, O.; Behmke, D. A.; Morris, J. D.; Simmons, R.; Anfuso, C.; Woodbridge, C. M.; Guo, Y. Adapting to the COVID-19 Online Transition: Reflections in a General Chemistry Sequence Taught by Multiple Instructors with Diverse Pedagogies. *J. Chem. Educ.* **2020**, *97* (9), 2458–2465.

(21) Wild, D. A.; Yeung, A.; Loedolff, M.; Spagnoli, D. Lessons Learned by Converting a First-Year Physical Chemistry Unit into an Online Course in 2 Weeks. *J. Chem. Educ.* **2020**, *97* (9), 2389–2392.

(22) Overview of ABINIT Tutorials. https://docs.abinit.org/tutorial/ (accessed Feb 2021).

(23) Tutorials. https://www.quantum-espresso.org/resources/ tutorials (accessed Feb 2021).

(24) High Performance Computing Facility. https://hpcf.umbc.edu (accessed Feb 2021).

(25) System Description. https://hpcf.umbc.edu/system-descriptiontaki/ (accessed March 2021).

(26) Giannozzi, P.; Baroni, S.; Bonini, N.; Calandra, M.; Car, R.; Cavazzoni, C.; Ceresoli, D.; Chiarotti, G. L.; Cococcioni, M.; Dabo, I.; Dal Corso, A.; de Gironcoli, S.; Fabris, S.; Fratesi, G.; Gebauer, R.; Gerstmann, U.; Gougoussis, C.; Kokalj, A.; Lazzeri, M.; Martin-Samos, L.; Marzari, N.; Mauri, F.; Mazzarello, R.; Paolini, S.; Pasquarello, A.; Paulatto, L.; Sbraccia, C.; Scandolo, S.; Sclauzero, G.; Seitsonen, A. P.; Smogunov, A.; Umari, P.; Wentzcovitch, R. M. QUANTUM ESPRESSO: A Modular and Open-Source Software Project for Quantum Simulations of Materials. *J. Phys.: Condens. Matter* **2009**, *21* (39), 395502.

(27) Giannozzi, P.; Andreussi, O.; Brumme, T.; Bunau, O.; Buongiorno Nardelli, M.; Calandra, M.; Car, R.; Cavazzoni, C.; Ceresoli, D.; Cococcioni, M.; Colonna, N.; Carnimeo, I.; Dal Corso, A.; de Gironcoli, S.; Delugas, P.; DiStasio, R. A.; Ferretti, A.; Floris, A.; Fratesi, G.; Fugallo, G.; Gebauer, R.; Gerstmann, U.; Giustino, F.; Gorni, T.; Jia, J.; Kawamura, M.; Ko, H. Y.; Kokalj, A.; Küçükbenli, E.; Lazzeri, M.; Marsili, M.; Marzari, N.; Mauri, F.; Nguyen, N. L.; Nguyen, H. V.; Otero-de-la-Roza, A.; Paulatto, L.; Poncé, S.; Rocca, D.; Sabatini, R.; Santra, B.; Schlipf, M.; Seitsonen, A. P.; Smogunov, A.; Timrov, I.; Thonhauser, T.; Umari, P.; Vast, N.; Wu, X.; Baroni, S. Advanced Capabilities for Materials Modelling with Quantum ESPRESSO. J. Phys.: Condens. Matter **2017**, 29 (46), 465901.

(28) Towns, J.; Cockerill, T.; Dahan, M.; Foster, I.; Gaither, K.; Grimshaw, A.; Hazlewood, V.; Lathrop, S.; Lifka, D.; Peterson, G. D.; Roskies, R.; Scott, J. R.; Wilkins-Diehr, N. XSEDE: Accelerating Scientific Discovery. *Comput. Sci. Eng.* **2014**, *16* (5), 62–74.

(29) Hohenberg, P.; Kohn, W. Inhomogeneous Electron Gas. *Phys. Rev.* **1964**, *136* (3B), B864–B871.

(30) Kohn, W.; Sham, L. J. Self-Consistent Equations Including Exchange and Correlation Effects. *Phys. Rev.* **1965**, *140* (4A), A1133–A1138.

(31) Mattsson, A. E.; Schultz, P. A.; Desjarlais, M. P.; Mattsson, T. R.; Leung, K. Designing Meaningful Density Functional Theory Calculations in Materials Science—A Primer. *Modell. Simul. Mater. Sci. Eng.* **2005**, *13* (1), R1–R31.

(32) Jones, R. O. Density Functional Theory: Its Origins, Rise to Prominence, and Future. *Rev. Mod. Phys.* **2015**, *87* (3), 897–923.

(33) Gettens, R. J.; Fitzhugh, E. W.; Feller, R. L. Calcium Carbonate Whites. *Stud. Conserv.* **1974**, *19* (3), 157–184.

(34) The Materials Project. https://materialsproject.org (accessed February 2021).

(35) Bennett, J. W.; Jones, D.; Huang, X.; Hamers, R. J.; Mason, S. E. Dissolution of Complex Metal Oxides from First-Principles and Thermodynamics: Cation Removal from the (001) Surface of $Li(Ni_{1/3}Mn_{1/3}Co_{1/3})O_2$. Environ. Sci. Technol. **2018**, 52 (10), 5792–5802.

(36) Bennett, J. W.; Jones, D. T.; Hamers, R. J.; Mason, S. E. First-Principles and Thermodynamics Study of Compositionally Tuned Complex Metal Oxides: Cation Release from the (001) Surface of Mn-Rich Lithium Nickel Manganese Cobalt Oxide. *Inorg. Chem.* **2018**, *57* (21), 13300–13311. (37) Bennett, J. W.; Jones, D. T.; Hudson, B. G.; Melendez-Rivera, J.; Hamers, R. J.; Mason, S. E. Emerging Investigator Series: First-Principles and Thermodynamics Comparison of Compositionally-Tuned Delafossites: Cation Release from the (001) Surface of Complex Metal Oxides. *Environ. Sci.: Nano* **2020**, *7* (6), 1642–1651.

(38) Abbaspour-Tamijani, A.; Bennett, J. W.; Jones, D. T.; Cartagena-Gonzalez, N.; Jones, Z. R.; Laudadio, E. D.; Hamers, R. J.; Santana, J. A.; Mason, S. E. DFT and Thermodynamics Calculations of Surface Cation Release in LiCoO₂. *Appl. Surf. Sci.* **2020**, *515*, 145865.

(39) Rong, X.; Kolpak, A. M. Ab Initio Approach for Prediction of Oxide Surface Structure, Stoichiometry, and Electrocatalytic Activity in Aqueous Solution. *J. Phys. Chem. Lett.* **2015**, *6* (9), 1785–1789.

(40) Huang, X.; Bennett, J. W.; Hang, M. N.; Laudadio, E. D.; Hamers, R. J.; Mason, S. E. Ab Initio Atomistic Thermodynamics Study of the (001) Surface of $LiCoO_2$ in a Water Environment and Implications for Reactivity under Ambient Conditions. *J. Phys. Chem. C* **2017**, *121* (9), 5069–5080.

(41) Tamijani, A. A.; Bjorklund, J. L.; Augustine, L. J.; Catalano, J. G.; Mason, S. E. Density Functional Theory and Thermodynamics Modeling of Inner-Sphere Oxyanion Adsorption on the Hydroxylated α -Al₂O₃ (001) Surface. *Langmuir* **2020**, *36*, 13166.

(42) Johnson, D. W.; Johnson, R. T. An Educational Psychology Success Story: Social Interdependence Theory and Cooperative Learning. *Educational Researcher* **2009**, *38* (5), 365–379.

(43) Hodges, L. C. Ten Research-Based Steps for Effective Group Work; IDEA, 2017.

(44) Bradley, S. M.; Middleton, A. P. A Study of the Deterioration of Egyptian Limestone Sculpture. *J. Am. Inst. Conserv.* **1988**, 27 (2), 64–86.

(45) Ryhl-Svendsen, M.; Glastrup, J. Acetic Acid and Formic Acid Concentrations in the Museum Environment Measured by SPME-GC/ MS. *Atmos. Environ.* **2002**, *36* (24), 3909–3916.

(46) Alebic-Juretic, A.; Sekulic-Cikovic, D. The Impact of Air Pollution on the Paintings in Storage at the Museum of Modern and Contemporary Art, Rijeka, Croatia. *Stud. Conserv.* **2009**, *54* (1), 49–57.

(47) Gibson, L. T.; Watt, C. M. Acetic and Formic Acids Emitted from Wood Samples and Their Effect on Selected Materials in Museum Environments. *Corros. Sci.* **2010**, *52* (1), 172–178.

(48) de la Fuente, D.; Vega, J. M.; Viejo, F.; Díaz, I.; Morcillo, M. Mapping Air Pollution Effects on Atmospheric Degradation of Cultural Heritage. *Journal of Cultural Heritage* **2013**, *14* (2), 138–145.

(49) Heimann, J. E.; Grimes, R. T.; Rosenzweig, Z.; Bennett, J. W. A Density Functional Theory (DFT) Investigation of How Small Molecules and Atmospheric Pollutants Relevant to Art Conservation Adsorb on Kaolinite. *Appl. Clay Sci.* **2021**, *206*, 106075.

(50) Vanderbilt, D. Soft Self-Consistent Pseudopotentials in a Generalized Eigenvalue Formalism. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1990**, *41* (11), 7892–7895.

(51) Garrity, K. F.; Bennett, J. W.; Rabe, K. M.; Vanderbilt, D. Pseudopotentials for High-Throughput DFT Calculations. *Comput. Mater. Sci.* **2014**, *81*, 446–452.

(52) Monkhorst, H. J.; Pack, J. D. Special Points for Brillouin-Zone Integrations. *Phys. Rev. B* **1976**, *13* (12), 5188–5192.

(53) Corum, K. W.; Huang, X.; Bennett, J. W.; Mason, S. E. Systematic Density Functional Theory Study of the Structural and Electronic Properties of Constrained and Fully Relaxed (0 0 1) Surfaces of Alumina and Hematite. *Mol. Simul.* **2017**, *43* (5–6), 406–419.

(54) Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996**, 77 (18), 3865– 3868.

(55) Wu, Z.; Cohen, R. E. More Accurate Generalized Gradient Approximation for Solids. *Phys. Rev. B: Condens. Matter Mater. Phys.* **2006**, 73 (23), 235116.

(56) Kokalj, A. Computer Graphics and Graphical User Interfaces as Tools in Simulations of Matter at the Atomic Scale. *Comput. Mater. Sci.* **2003**, *28* (2), 155–168.

(57) Momma, K.; Izumi, F. VESTA 3 for Three-Dimensional Visualization of Crystal, Volumetric and Morphology data. *J. Appl. Crystallogr.* **2011**, 44 (6), 1272–1276.