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COUNCIL ON UNDERGRADUATE RESEARCH

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CUR Focus

Developing a Regional Computational Chemistry Consortium Through Undergraduate Research Conferences

The Midwest Undergraduate Computational Chemistry Consortium (MU3C) is a community of 14 computational chemistry professors and their undergraduate research collaborators at 11 colleges and universities. The professors in the consortium are engaged in a wide variety of computational research projects, as well as experimental research programs, on the 11 campuses (see Table 1).

Our consortium's most important activity is an annual regional undergraduate research (UR) conference focused on oral and poster research presentations by our students. These annual summer meetings, hosted by Midwestern research universities, provide valuable research training for our students, foster the development of relationships among students and professors, and have helped the consortium obtain two instrumentation grants from the National Science Foundation (NSF). The development of MU3C and what we believe are the advantages of our meeting format may prove instructive for other campuses.

Context and Our Inaugural Meeting

It is rare for a chemistry department at a primarily undergraduate institution (PUI) to have more than one faculty member whose specialty is computation and molecular modeling. That professor and his or her students thus lack regular opportunities to interact with colleagues who take other approaches to computational chemistry. Attending American Chemical Society meetings or Gordon Conferences provides PUI computational chemists and their research students some relief from this intellectual isolation. However, these meetings tend to be expensive, and even regional meetings provide few opportunities for undergraduates to present their research. According to the Survey of Undergraduate Research Experiences sponsored by the Howard Hughes Medical Institute, students rate final presentations as one of the most valuable components of a summer research program, and the opportunity to present one's work formally is correlated with self-reported learning gains in both speaking and writing about science (Lopatto 2007). Giving a research

Table 1. Current Members of the Midwest Undergraduate Computational Chemistry Consortium

Faculty Member	Institution	Primary Computational Research Interest
Erin Dahlke Speetzen	University of Wisconsin-Stevens Point	Substituent effects on phenyl shifts
Scott E. Feller	Wabash College	Membrane dynamics and force field development
Jason G. Gillmore	Hope College	Reduction potentials and excited state energies of organic dyes
Heriberto Hernandez-Soto	Grinnell College	Heterogeneous processes in the atmosphere and materials
Daniela Kohen	Carleton College	Adsorption and diffusion within molecular sieve materials
Brent P. Krueger	Hope College	Models of fluorescence-detected resonance energy transfer
Keith T. Kuwata	Macalester College	Reactions of chemically activated atmospheric species
Christopher P. Lawrence	Grand Valley State University	Dynamics of tropospheric aerosols and biomolecules
Maria C. Nagan	Truman State University	RNA structure and recognition
Eric V. Patterson	Truman State University	Reaction dynamics of phosphonothiolates
William F. Polik	Hope College	Highly accurate potential energy surfaces and spectroscopy
Joseph D. Scanlon	Ripon College	Silver-based catalysts for C-H bond amination reactions
Jonathan M. Smith	Temple University	Collisional dynamics of radicals and small organics
Stacey A. Stoffregen	University of Wisconsin-River Falls	Photochemistry of aromatic sulfoxides and selenoxides

A group of MU3C students and faculty members after a day of talks at the 2005 summer meeting hosted by the University of Minnesota-Twin Cities.

presentation to an audience that shares the presenter's specific disciplinary interests provides the added benefit of detailed and relevant feedback.

A decade ago this situation inspired the authors, each of whom is a computational chemist at a PUI in the Upper Midwest, to form a consortium committed to organizing annual meetings centered on undergraduate research talks. To provide a richer intellectual experience for both ourselves and our students, we sought to locate our meetings at Midwestern research universities that house vibrant computational chemistry programs. Professors Mark Ratner and Tamar Seideman of Northwestern University hosted our inaugural meeting in August 2003. Our hosts listened to talks from seven undergraduates and gave informal overviews of their own research programs. Northwestern professors, graduate students, and postdoctoral fellows provided an extensive tour of their computational and experimental facilities, and engaged with us during talks, at meals, and at other social events.

Our first meeting was a success. Our students all reported being stimulated by their exposure both to the Northwestern computational chemistry program and to the diversity of research interests and techniques pursued by the consortium's four founding faculty members. Students also appreciated the opportunity to talk about their chemistry projects and to ask questions about other people's in a nonthreatening environment. Our Northwestern hosts likewise found the experience worthwhile. One wrote soon after the meeting, "I very much enjoyed the opportunity to talk with some of your students and was impressed by the talks that they presented both in terms of the science and in terms of the presentation. I have many years of (always delightful) experience in working with undergraduate students and hence I do have a 'standard' to compare with." Finally, the MU3C faculty members enjoyed the opportunities to share stories and ideas about the challenges of teaching and doing research at small PUIs.

Development of MU3C Meetings

Our positive experiences at Northwestern in 2003 reinforced our commitment to meet at a research university every summer and to follow the same student-focused format. Table 2 summarizes data about these meetings, which last from two to three days depending on the number of student presentations. Participation by the consortium's member faculty has varied somewhat over the years, largely as a consequence of professional or life events such as sabbaticals, moving to different institutions, or the birth of children. Nevertheless, each meeting since 2003 has included students from at least one institution besides those of the consortium's founders (Carleton, Hope, and Macalester Colleges). Moreover, students, the consortium's participating faculty, and professors at the hosting university continue to report high levels of satisfaction about each meeting.

As Table 2 indicates, we have met in the Midwest every summer except in 2008. One reason for our geographic focus is to keep travel relatively inexpensive. We believe strongly in the intellectual benefits provided by our UR meetings, and we are committed to providing an opportunity for each of our research students to experience these benefits. While most of our member campuses provide some financial support for students and their mentors to attend professional meetings, the amount of funding is limited. Keeping meetings within driving distance of most MU3C campuses is therefore desirable.

The second reason for our Midwestern focus is our interest in building strong and enduring relationships among a relatively small number of computational chemistry professors and students. For example, we have met twice at Northwestern (in 2003 and 2009), twice at UW-Madison (2004 and 2010), and we will return to Minnesota for our 2012 meeting. The positive impressions formed by a MU3C meeting benefit both our undergraduates seeking admission to top graduate chemistry programs and graduate faculty members seeking talented and motivated students. For example, two MU3C students who presented at the 2009 meeting at Northwestern have since entered graduate studies there. In addition, collaborations between researchers at consortium members and faculty at the hosting institutions develop more naturally because of proximity. For example, a MU3C student started a research collaboration with Iowa State University chemist Mark Gordon soon after the 2006 meeting that Professor Gordon had hosted.

The consortium's annual meetings are organized to allow all students to present their work. With the growth of our consortium, however, the number of student presentations would be too large to fit into a two- or three-day meeting if every individual gave a talk. Therefore, in our current structure, more experienced students give talks, some individually and some in pairs or groups of three if their projects have

Table 2. Participation at MU3C Undergraduate Research Meetings

Year	Hosting Institution	Number of Participating MU3C Research Groups	Number of Students Giving Presentations
2003	Northwestern University	4	7
2004	University of Wisconsin-Madison	5	9
2005	University of Minnesota-Twin Cities	8	24
2006	Iowa State University	8	15
2007	University of Illinois at Urbana-Champaign	6	14
2008	Hamilton College (MERCURY Conference)	4	10
2009	Northwestern University	9	20
2010	University of Wisconsin-Madison	5	6
2011	University of Chicago	11	21

significant overlap. Students engaged in their first summer of research are encouraged to present a poster instead of giving a talk. Having a poster session breaks up the schedule and provides valuable opportunities for informal scientific discussions. Research talks from faculty members at the hosting institution and laboratory tours provide students additional opportunities to discuss and explore new scientific ideas.

While the principal focus of our meetings is the student experience, MU3C faculty members also use consortium meetings for professional development. The relatively small size of our consortium has made it easy for the participating faculty members to get to know and trust one another. We have discussed issues such as incorporating computational chemistry into our departmental curricula, getting research done in spite of sizable teaching loads, navigating campus politics, and tackling specific computational chemistry challenges. This mutual professional mentoring has been valuable not only for tenure-track faculty members, but also for tenured faculty members who lack adequate professional support at their home institutions (Karukstis 2010).

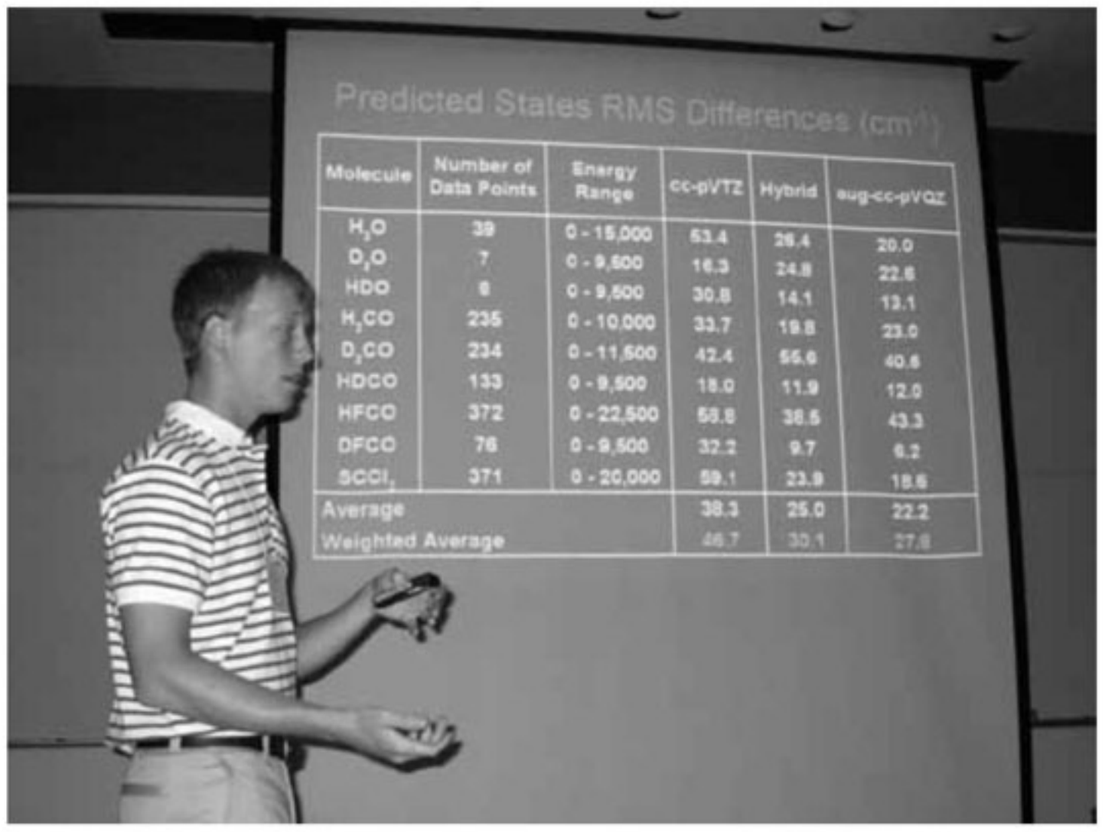
Another regular part of each meeting is a panel discussion for graduate students and post-doctoral fellows at the host research institution who are interested in teaching at a PUI. Dozens of people attend this discussion every year. The major points we convey to our potential future colleagues are the near ubiquity of research expectations at PUIs (Elrod, Husic, and Kinzie 2010) and the heterogeneity of our experiences as faculty members regarding issues such as teaching load, the need to publish research in peer-reviewed disciplinary journals, and the need to pursue and secure research grants.

The profitable and enjoyable interactions among MU3C students and professors at our annual meetings have inspired us to pursue ways to sustain these relationships throughout the year. Thus we have engaged in other formal community-building activities such as online conferences and the writing of proposals for National Science Foundation grants. All of these activities have contributed to student learning, faculty development, and research progress. These are benefits common to intentionally developed undergraduate research communities (Bender, Blockus, and Webster 2008).

Online Conferences

The main goals of our online conferences are to give our student researchers the opportunity to provide updates on the research they have been conducting since the summer meeting and to maintain relationships formed during previous in-person meetings. Our first online conference, in February 2004, featured nine students presenting either posters in Adobe pdf format or using sets of Microsoft PowerPoint slides. All MU3C students and faculty members were expected to post at least one question or comment about each presentation, with the goal of sparking further discussion. By the end of the online conference, participants had submitted more than 140 posts. This winter online meeting has become a MU3C annual tradition.

The online conferences encourage students to make progress on their research projects during the fall term and to deepen their understanding of their work in the way that preparing presentations always does for any scholar. The online format gives students (and professors) the freedom to ask very basic questions about the concepts and techniques underlying each project. This has been useful for experimental colleagues who have the desire, but not necessarily the technical background, to incorporate computation into their research programs. Moreover, unlike the situation at an in-person poster session, all participants can benefit simultaneously from the informative dialogue. Our 2012 online conference featured 21 presentations from 12 different research groups, and involved 51 student and faculty participants. It generated 211 posts.



John Davisson of Hope College gives a talk on work he did in collaboration with Professor William F. Polik at the 2005 summer MU3C meeting at the University of Minnesota-Twin Cities.

Finally, the consortium's online meetings have been an effective outreach tool. Students working for Professors Erin Dahlke Speetzen (University of Wisconsin-Stevens Point), Scott Feller (Wabash College), and Stacey Stoffregen (University of Wisconsin-River Falls) all presented at an online meeting before attending a summer in-person meeting. Over the years we have also had a number of students and professors who have participated in the online conference strictly as observers. These observers have been able to get a flavor of the breadth and quality of computational chemistry research being pursued by MU3C members.

NSF Instrumentation Proposals

Getting together twice a year (once in person and once online) clearly provides MU3C students better research training in computational chemistry than if they remain isolated on their home campuses or if they attended only generic professional meetings. Another way to improve research training for our students is to provide them with state-of-the-art computer equipment on which they can run their calculations. Having such resources benefits our chemistry students in general by allowing MU3C faculty members to increasingly integrate computation into our institutions' chemistry curricula.

However, because most PUIs have at most one computational chemist, these institutions rarely perceive a need to provide significant scientific computing resources. Start-up funds and external grants, if available, enable a junior faculty member to purchase a modest computer cluster, but using a small cluster to perform highly accurate quantum chemical calculations or run long molecular dynamics simulations on realistically sized systems is either impossible or very time consuming. The National Science Foundation's Extreme Science and Engineering Discovery Environment project offers professors at PUIs the opportunity to apply for access to state-of-the-art computers. However, even if a successful supercomputing proposal gains a faculty member adequate computer time to pursue a project, long wait times in queuing systems impede research progress. This can be particularly frustrating in the PUI context, in which research students accomplish most of their work during a ten-week summer session. The great difficulty, if not impossibility, of temporarily reserving large numbers of processors also makes using NSF computational resources impractical for conducting computational chemistry exercises in a lecture-based classroom or in a laboratory setting.

Shortly after its inception, MU3C members realized that the scientific community we had begun to build by means of our undergraduate research meetings could be leveraged to obtain high-performance computing hardware, which in turn had the potential to increase the quality and quantity of the results our students presented at subsequent meetings. We therefore decided to seek funding for a cluster computer from the NSF Major Research Instrumentation (MRI) program in 2005. The MRI proposal not only sought to demonstrate the scientific significance and productivity of our individual research programs, but also made the case for the impact our annual meetings had on students' research training. We were fortunate to receive letters of support from both past and future research university hosts that expressed their enthusiasm and high regard for our annual summer conferences.

Our 2005 proposal was successful, with almost $380,000 being awarded to Hope College, which had agreed to house and maintain the new computer cluster. The proposal reviews indicated that our annual UR meetings had made our funding request more persuasive. One reviewer wrote, "Bringing undergraduates associated with the MU3C consortium together at major graduate institutions such as Northwestern and Iowa State is a stroke of genius, and I predict that many other Midwestern graduate institutions will be trying to convince MU3C to allow them to be hosts. These conferences will have a profound impact on the undergraduates in exposing them to graduate research, graduate students, and chemistry faculty at the host institutions."

The MRI-funded computer cluster soon became an important research and teaching tool for most MU3C professors. As we gained more consortium members, and as our students sought to run more ambitious calculations, however, we began to tax the cluster's capacity. By 2009, the average calculation had to wait in a queue for 24 hours before starting to run, and one-third of calculations needed at least two weeks to finish. It was time to seek funding for a new cluster. After an unsuccessful attempt in 2009, we secured a $300,000 grant in 2010. Reviewers again viewed our annual UR meetings positively. The review panel's summary stated, "The annual meetings will expose students and faculty to multiple computational approaches and foster mentoring among undergraduates, MU3C faculty, and faculty and students at the hosting universities."

Apart from the obvious benefit of having state-of-the-art computer hardware with which to conduct research, the process of writing three MRI grant proposals has had a positive impact on our UR meetings. First, before submitting each proposal, MU3C faculty members have sought commitments from our deans or provosts to defray the costs of travel, lodging, and meals for our summer meetings during the lifetimes of each grant. Most of us have obtained such commitments. This has not only given us an important fact to highlight in our proposals, but has also helped ensure a good number of participants at each meeting.

Second, reviewers of our last two proposals wanted to see slightly stronger student publication records. We agree that it is not enough to keep our research students busy running calculations that will enable them to give presentations at MU3C conferences. We must always strive to engage our students in research that is significant enough to be published in peer-reviewed journals. It is this caliber of research that provides students with the best scientific education (Gavin 2000). Moreover, during our meetings, we should be intentional about providing our students and each other the kind of specific, insightful feedback that will help us get work published in top journals.

Finally, reviewers of all three proposals have enthusiastically affirmed that the structure of our annual UR meetings is highly beneficial to our students. This is consistent with the positive feedback we have heard from students and research university colleagues over the years.

Concluding Remarks

Our current challenge as a consortium is to preserve what is good about MU3C meetings as we continue to grow. We could accommodate a large increase in the number of student participants if a majority of them gave posters. It would still be essential for at least one student from each research group to give a talk on his or her work. Second, we are small enough to be flexible in our scheduling. In years when there is a high demand for student talks, we can meet over three days instead of only two days and schedule fewer talks from faculty members at the hosting institution.

Ultimately, the size of our consortium and the number of students and professors attending any one meeting will likely reach a natural limit. Our geographical focus remains in the Midwest, and it is unlikely that computational chemists from other parts of the country will start coming to our meetings regularly. Moreover, other consortia, such as MERCURY (the Molecular Education and Research Consortium in Undergraduate Computational Chemistry), and MoleCVUE (Molecular Computation and Visualization in Undergraduate Education), ably serve PUI computational chemists with their annual meetings. MERCURY meetings, led by Bucknell University Provost George Shields, engage PUI students and faculty members with plenary talks by top computational chemists from academia, national laboratories, and industry. MoleCVUE meetings, currently chaired by Professor Carl Salter of Moravian College, focus on the teaching and research interests of the PUI faculty members in attendance.

MU3C faculty members have multiple connections with faculty members in these other consortia, including collaborations on NSF grants, joint organization of sessions at American Chemical Society national meetings, and attendance at MERCURY and MoleCVUE meetings. Being an effective computational chemist at a PUI is a multidimensional challenge, and each of our consortia helps professors achieve different professional goals. The Midwest Undergraduate Computational Chemistry Consortium remains committed to providing excellent research training for our undergraduate collaborators. Evidence shows that our annual regional undergraduate research meetings play a major role in that training.

References

Bender, Carol, Linda Blockus, and Marcus Webster. 2008. "Creating Community in Your Undergraduate Research Program: It isn't Spontaneous!" *CUR Quarterly* 28(4):8-12.

Elrod, Susan, Diane Husic, and Jillian Kinzie. 2010. "Research and Discovery across the Curriculum." *Peer Review* 12(2):4-8.

Gavin, Robert. 2000. "The Role of Research at Undergraduate Institutions: Why is it Necessary to Defend It?" In *Academic Excellence: The Role of Research in the Physical Sciences at Undergraduate Institutions,* edited by Michael P. Doyle, 9-16. Tucson, AZ: Research Corporation.

Karukstis, Kerry K. 2010. "A Horizontal Mentoring Initiative for Senior Women Scientists at Liberal Arts Colleges." *CUR Quarterly* 31(2):33-39.

Lopatto, David. 2006. "Undergraduate Research Experiences Support Science Career Decisions and Active Learning." *CBE-Life Sciences Education* 6:297-306.

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Keith T. Kuwata is a professor of chemistry at Macalester College in Saint Paul, Minnesota, where he has taught since 2000. Kuwata first experienced undergraduate research while studying chemistry at Harvey Mudd College in Claremont, California, where he earned his BS in 1991. He earned a PhD in chemistry from the California Institute of Technology in 1998 and then served as a postdoctoral scholar and lecturer at the University of California, Los Angeles for two years before beginning his position at Macalester. Kuwata and his students have published nine

papers using computational chemistry to characterize the reactivity of transient species in the lower atmosphere.

Daniela Kohen is an associate professor of chemistry at Carleton College in Northfield, Minnesota, where she has taught since 2002. She received her licenciatura en ciencias químicas from Universidad de Buenos Aires in 1990 and her PhD in chemical physics from the University of Notre Dame in 1995. She did postdoctoral work at Bell Laboratories, Lucent Technologies, and the University of California at Irvine, and taught at Smith College before going to Carleton. Kohen's general research area is in condensed phase dynamics. Currently, she and her students are using atomistic simulations to understand and characterize how small gas molecules interact with pure CO_2.

Brent P. Krueger is an associate professor of chemistry at Hope College in Holland, Michigan, where he began teaching in 2001 following a brief postdoctoral research appointment at the Free University in Amsterdam and an NIH postdoctoral fellowship at the University of California at San Francisco. He earned his PhD in physical chemistry from the University of Chicago after earning his undergraduate degree in chemistry and physics from Truman State University. His research program is in biophysics. Krueger and his students seek to harmonize experimental results from fluorescence spectroscopy with the results of molecular dynamics and quantum mechanics computer simulations.

William F. Polik is the Edward and Elizabeth Hofma Professor of Chemistry at Hope College. He has been named a Fellow of both the American Association for the Advancement of Science and the American Chemical Society. Early in his career he received an NSF Presidential Young Investigator award. He has involved more than 60 undergraduate students in his research program at Hope, of whom 25 are co-authors on publications. He is co-developer of WebMO, a web-based interface for computational chemistry, which is in use at more than 1,400 academic and research institutions worldwide. Polik has chaired both the Beckman Scholar Program's Executive Committee and the American Chemical Society's Committee on Professional Training during its development of new guidelines for undergraduate chemistry programs. He received his PhD in physical chemistry from the University of California, Berkeley, in 1988 after graduating from Dartmouth College in 1982.

UNDERGRADUATE RESEARCH AND CHANGE IN HIGHER EDUCATION: A SCHOLARLY DISCUSSION
Pre-ISSOTL Workshop, Hamilton Ontario, October 24, 2012
8:30AM-4:00PM

This day-long symposium will explore how undergraduate research effects change in higher education, and how a variety of changes in higher education affect undergraduate research.

Workshop subthemes include:

- Students as change agents
- Undergraduate research generating transformative learning
- The role of undergraduate research in curriculum renewal
- The influence of technological changes on undergraduate research
- The influence of changing student demographics on undergraduate research
- Supporting and sustaining undergraduate research in times of fiscal challenge

The expected outcomes for participants include:

- A raised awareness of the possibilities of undergraduate research to transform both student and institutional learning
- Consideration of how technology can support and enhance undergraduate research
- Practical advice regarding how to change a curriculum to embed undergraduate research
- The sharing and showcasing of good practice in undergraduate research
- The facilitation of networks amongst staff and students interested in undergraduate research
- The option of joining a collaborative group to continue working on undergraduate research

Workshop attendees are invited to present posters highlighting undergraduate research efforts on their own campuses that are focused on the theme and subthemes of the symposium. The poster submission deadline is September 1, 2012. Information regarding submission instructions is available at www.cur.org/pre-ISSOTLposter.html.

For more information and to register visit: http://issotl12.com/cur-workshop/.