Twenty Years of Exceptional Success: The **M**olecular **E**ducation and **R**esearch **C**onsortium in **U**ndergraduate computational chemist**RY** (**MERCURY**)

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**Abstract**

The MERCURY consortium, established in 2000, has contributed greatly to the scientific development of faculty and undergraduates. The MERCURY faculty peer review publication rate from 2001-2019 of 1.7 papers/faculty/year is 3.4 times the rate of physical science faculty at primarily undergraduate institutions. We have worked with over 1000 students on research projects since 2001, and 75% of our undergraduate research students have been underrepresented in chemistry, either female or students of color. Approximately half of our alumni attend graduate school for the purpose of obtaining advanced degrees in STEM fields and 2/3 are female and/or students of color. We have had more than 1600 attendees at the 18 MERCURY conferences, including 111 invited speakers, 61 of whom have been female and/or faculty of color. In this paper the research accomplishments, transformational outcomes, and scientific productivity of the MERCURY faculty are highlighted.

**Keywords:** *consortium, diversity, females in STEM, high-impact practices, inclusion, MERCURY, NSF-MRI, scientific excellence, students of color in STEM, undergraduate research*

1. **Introduction**

The MERCURY consortium was formed during the 1999-2000 academic year, and a history of the evolution of the consortium has been published.[1](#_ENREF_1) That paper traced how the consortium grew from seven faculty at liberal arts colleges in the Northeast in 2001, when the first National Science Foundation (NSF) Major Research Instrumentation (MRI) grant was received to support the consortium, to 27 faculty at predominately undergraduate institutions (PUIs) in 2019. It also detailed the huge impact the annual MERCURY conference has on the productivity of our undergraduate research groups. In the Fall of 2019 we invited more faculty into the consortium, so we are now 38 faculty working with undergraduate research groups at 33 institutions across the country. MERCURY has been supported by five NSF MRI grants, as well as internal funds from Hamilton College, Armstrong Atlantic State University, Bucknell University, and Furman University to support hosting the shared computational resources and the annual conferences, and by all the colleges and universities in the consortium who have committed to paying for their faculty and students to attend the annual meeting. In this paper I will outline the scientific productivity, both in terms of research accomplishments and transformational outcomes, that the first five NSF MRI grants enabled and then highlight the ongoing research efforts of the 38 MERCURY faculty in the consortium today. Research Accomplishments and Transformational Outcomes align with the NSF criteria for grant funding, which are Intellectual Merit and Broader Impacts

1. **Research Accomplishments (Intellectual Merit) and Transformational Outcomes (Broader Impacts) of the Five MERCURY NSF MRI Proposals**

**2.1 First NSF-MRI Award, August 28, 2001, $400,000, CHE-0116435**

“Acquisition of High Performance Computers for the Northeastern Undergraduate

Research Chemistry Consortium”

*Research Accomplishments*

The seven faculty who started the consortium were **Jeffery Greathouse** (*St. Lawrence*, environmental), **Maria Gomez** (*Vassar*, materials), **Carol Parish** (*Hobart & William Smith*, physical organic), **Ramona Taylor** (*Holy Cross*, environmental and materials), **Martha Reynolds**(*Colgate*, bioinorganic), **Marc Zimmer** (*Connecticut*, bioinorganic) and **George Shields** (*Hamilton*, biophysical). Over the three-year grant period, the seven faculty and their students published 44 research papers in peer-reviewed journals with their students.[2-45](#_ENREF_2) This equates to two published papers per year per faculty member, which is four times higher than the usual productivity of a faculty member at a predominately undergraduate institution (PUI) as documented by Research Corporation.[46](#_ENREF_46) Further, in the first four years after the consortium was established, the number of external grant awards received by the faculty more than tripled and the MERCURY investigators raised more than four million dollars to support computational chemistry research involving undergraduate students. The bulk of this funding was used to provide summer stipends, which allowed students to be immersed fulltime in research. Mentoring provided by senior researchers to junior researchers, and networking at the national meeting, have contributed greatly to the high rate of success in recruiting and retaining students, particularly those from underrepresented groups. The seven MERCURY investigators worked with more than 110 undergraduates on research projects during the first three-year grant period. Marc **Zimmer**’s *Chemical Reviews* article on Green Fluorescent Protein has been cited over 770 times in the Web of Science database (WOS).[41](#_ENREF_41) Maria **Gomez**’s *PNAS* paper on the hydration and mobility of aqueous OH- has been cited more than 130 times in WOS.[5](#_ENREF_5) The **Shields** lab work on pKa calculations invigorated the field, with two *JACS* papers cited more than 440 times each,[20](#_ENREF_20), [24](#_ENREF_24) and two other research papers cited more than 140 times each in WOS.[19](#_ENREF_19), [23](#_ENREF_23) Similarly, the lab’s *JACS* paper on water clusters in the atmosphere has been cited more than 130 times.[26](#_ENREF_26)

*Transformational Outcomes*

This proposal requested $780,220 from NSF, matched with $400,000 by Hamilton College, and $215,000 from the Consortium Colleges, to support the acquisition of high-end computers for the seven researchers and their students. The consortium purchased two workstations for each institution to serve as local graphics and a 32 processor Origin 300 and an 8 processor Origin 300 located at Hamilton College. In addition, we built a 30-node Beowulf Cluster for the consortium. We used NSF funds to hire a System Administrator and we organized an annual conference for any and all undergraduates to present their work in computational chemistry, to learn from our invited speakers, and to network with other students and faculty in attendance. The consortium has attracted many more women into this traditionally male-dominated research area. Three of our research groups consisted of at least 40% African-American or Hispanic-American students. This proposal had a particularly positive impact on the careers of Maria **Gomez** and Carol **Parish**. **Gomez** moved from Vassar College to Mt. Holyoke College in 2003 and is currently the *Elizabeth Page Greenwalt Chair in Physical Sciences*. She was awarded a Henry Dreyfus Teacher-Scholar Award in 2007. She directs the Passport to Chemistry Adventure program supported by Dreyfus. **Parish** moved from Hobart & William Smith Colleges to the University of Richmond in 2005, where she is the *Floyd D. and Elisabeth S. Gottwald Chair in Chemistry*. She is the recipient of numerous awards throughout her career, including the Henry Dreyfus Teacher-Scholar Award (2005), the ACS Stan Israel Award for Advancing Diversity in the Chemical Sciences (2011), the Council on Undergraduate Research Goldwater Mentor Award (2016), the ACS Committee on Minority Affairs Zaida C. Morales-Martinez Prize for Outstanding Mentoring of ACS Scholars (2017), and the ACS Award for Research at an Undergraduate Institution (2019).

**2.2 Second NSF-MRI Award, August 3, 2005, $100,000, CHE-0521063**

“Acquisition of a Linux Cluster for the Molecular Education and Research Consortium in

Undergraduate computational chemistry (MERCURY)”

*Research Accomplishments*

Undergraduate faculty **Maria Nagan** (*Truman State,* biochemistry), **Glênisson de Oliveira** (*Rhode Island College*, physical), **Wingfeld Glassey** (*Hobart & William Smith,* physical), and **Tricia Shepherd** (*Westminster College, Utah*, physical) joined **Gomez**, **Parish**, **Shields**, and **Zimmer**, while Reynolds, Greathouse, and Taylor left the consortium, as did Glassey before the end of the grant period. The PI invited five additional investigators into the consortium during the grant period: **Mauricio Cafiero** (*Rhodes College*, biochemistry), **Kelling Donald** (*University of Richmond*, chemical bonding), **Becky Eggimann** (*Wheaton College, IL*, solvation), **Daqing Gao** (*Queensborough Community College of CUNY*, physical organic), and **Eric Patterson** (*Truman State*, physical organic). These MERCURY investigators published 50 papers,[47-96](#_ENREF_47) which translates to 1.9 publications/faculty/year (seven faculty were in the consortium for three years; five were in the consortium for one year). This is 3.8 times the national average (0.5 pubs/faculty/year).[46](#_ENREF_46)

*Transformational Outcomes*

The 12 MERCURY consortium PIs worked with 140 undergraduate students, 13 high school students, 7 high school teachers, and 6 senior scientists at their institutions over the three-year grant period. Of the 140 undergraduates, 89 were female, 14 were Asian, 13 were Black or African-American, and 12 were Hispanic or Latino. A total of 101 undergraduates were female and/or students of color, which is 72% of the undergraduates trained in our labs. Our students won twenty national or international awards such as Goldwater Scholarships and Fulbright Fellowships during this period. We hosted three more MERCURY conferences in the summers of 2006, 2007, and 2008, with a total of 251 participants. Over seventy-five percent of the participants were undergraduates or high school students. Over fifty percent of the speakers and fifty percent of the participants were women or people of color.

**2.3 Third NSF-MRI Award, July 15, 2008, $229,000, CHE-0521063, CHE-1044256** “Acquisition of a High Performance Computer for the Molecular Education and Research Consortium in Undergraduate computational chemistry (MERCURY)”

*Research Accomplishments*

Both **de Oliveira** and **Gao** left the consortium and Clifford **Padgett** (*Armstrong Atlantic State University*, biochemistry) and **Adam Van Wynsberghe** (*Hamilton*, biochemistry) were invited into the consortium in the second year of the grant. MERCURY faculty published 62 publications during the third MRI grant period,[97-158](#_ENREF_97) for an average number of 1.7 papers published per investigator per year, a rate 3.4 times the average rate at PUIs.[46](#_ENREF_46) The **Shields** lab’s papers on water clusters have been cited over 150 and 185 times,[131](#_ENREF_131), [143](#_ENREF_143) and their review article on pKa calculations cited over 125 times.[129](#_ENREF_129)

*Transformational Outcomes*

This proposal funded $229,000 for an SGI Altix 450. The 13 MERCURY investigators worked with 165 undergraduates over the three years of this grant. Of the 13 MERCURY investigators, five are female; and of the 13, three are Hispanic, one is Asian, and one is Black. The diversity of the PIs as well as their overall commitment to inclusion of all interested students in their work is reflected in their work with their undergraduate research assistants. A total of 197 personnel worked on this project as a result of this award. This includes three other senior researchers/technicians, five postdoctoral associates (one Asian female, a Black female, and a Black male), 165 undergraduates, three high school students, 11 pre-college teachers, and one post-baccalaureate fellow. Of the 165 undergraduates, 92 were female (55%), 26 of the 165 were Asian (16%), 21 were Black (13%), and nine were Hispanic (5%). Of the 92 females, 14 were Asian, 13 were Black, and two were Hispanic. Thus 34% of the undergraduate student researchers were students of color. Including all female students and male students of color, 119 of the 165 were female and/or students of color, which is 72% of the total.

**2.4 Fourth NSF-MRI Award, August 22, 2012, $200,000, CHE-1229354**

“MRI: Acquisition of High Performance Computers for the Molecular Education and Research Consortium in Undergraduate computational chemistry (MERCURY)”

*Research Accomplishments*

**Padgett** left the consortium, **Gao** (*Central State***)** rejoined, and **Kelly Anderson** (*Roanoke College*, physical), **Aimée Tomlinson** (*North Georgia College*, physical), **Sudeep Bhattacharyay** and **Jim Phillips** (*University of Wisconsin-Eau Claire*, biophysical & physical) joined, bringing the total to 17 MERCURY investigators. We published 79 peer-reviewed papers,[159-237](#_ENREF_159) or 1.5 papers/faculty/year, which is three times the rate for physical science faculty at undergraduate institutions.[46](#_ENREF_46) The **Shields** group’s collaboration with Brooks Pate resulted in a *Science* paper on the structures and energetics of the gas-phase water hexamer,[160](#_ENREF_160) which has been cited over 250 times. They showed conclusively that three (H2O)6 isomers are formed in a low temperature beam, and that the Cage is the lowest energy isomer.[160](#_ENREF_160) **Patterson** published a paper in *Science* on the fate of metabolites of the steroidal growth promoter, trenbolone acetate, which is administered to beef cattle. Based on the chemistry they concluded that predictive models and risk assessment must take into account the transformation products of high-risk environmental contaminants such as endocrine-disrupting steroids.[184](#_ENREF_184) **Parish** and **Donald** published a paper in *JACS* on halogen bonding in DNA base pairs,[169](#_ENREF_169) which has been cited over 70 times in WOS.

*Transformational Outcomes*

During the three-year period of this grant, the 17 MERCURY investigators worked with 200 undergraduates, and over 75% of them were female and/or from underrepresented groups. In addition, 16 high school students, 2 post-baccalaureate alumni, 2 technicians, 4 post-doctoral researchers, and a staff research scientist worked with the MERCURY investigators.

**2.5 Fifth NSF-MRI Award, September 1, 2016, $225,000, CHE-1626238, 1662030** “MRI: Addition of High Performance Computers for the Molecular Education and Research Consortium in Undergraduate computational chemistry (MERCURY)”

*Research Accomplishments*

Undergraduate faculty **George Barnes** (*Siena*, physical), **Chrystal Bruce** (*John Carroll*, physical), **Nick Boekelheide** (*Colby*, biophysical), **JiaJai Dong** (*Bucknell*, biophysics), **Dmitri Kosenkov** (*Monmouth*, physical), **Ashley Ringer McDonald** (*Cal Poly*, biophysical), **Bill Miller III** (*Truman State*, biochemistry), **Juan Navea** (*Skidmore*, physical), **Joshua Schrier** (*Haverford*, Physical), **Isaiah Sumner** (*James Madison*, biochemistry), and **Mychel Varner** (*Iona,* physical) joined the consortium in 2016. **Boekelheide** left in 2017 for family reasons and in 2017-18 we added **Heidi Hendrickson** (*Lafayette College*, Physical), **Kedan He** (*Eastern Connecticut State University*, biological), **Aurelia Ball** of (*Skidmore College*, biochemistry), and **Joseph Baker** (*The College of New Jersey*, biochemistry). In 2018 Marc **Zimmer,** one of the original senior investigators, retired from the consortium. **Eggimann** and **Gao** left the consortium as well, bringing us to 27 faculty at 24 different institutions. The faculty published two peer-reviewed books,[238-239](#_ENREF_238) 9 peer-reviewed book chapters,[240-248](#_ENREF_240) and 115 peer-reviewed research papers.[249-363](#_ENREF_249) This comes to 1.6 peer-reviewed products/faculty/year during the three-year grant period, which is 3.2 times the rate of publication for natural science faculty at PUIs.[46](#_ENREF_46)

*Transformational Outcomes*

Overall, during the 2016-19 grant period we worked with 325 undergraduates, and 71% were female and/or students of color. In addition, 9 high school students, 2 post-baccalaureate fellows, 3 master’s students, 2 post-doctoral researchers, and a staff research scientist worked with the MERCURY investigators. We held four successful conferences, averaged 102 attendees with an average of 52.5 undergraduate poster presentations. Of our 24 speakers, 16 were female and/or faculty of color. We held pre or post- conference MolSSI programming workshops each summer. **Shields** is on the MolSSI Science & Software Advisory Board. **McDonald** and **Ball** are both MolSSI associates, and are well known for their development of undergraduate programming curriculum and MolSSI workshops.

**2.6 Summary of Impacts, 2001-2019**

*Research Accomplishments (Intellectual Merit)*

One of the challenges to the overall undergraduate research movement is that the ability of undergraduate research to advance scientific knowledge remains undervalued.[364-365](#_ENREF_364) From 2001, when the first NSF-MRI grant was funded, through the summer of 2019, the MERCURY investigators have published 361 peer-reviewed publications, including two in *Chemical Society Reviews*,[104](#_ENREF_104), [269](#_ENREF_269) one in *Chemical Reviews*,[41](#_ENREF_41) one in *Nature Reviews Chemistry*,[*328*](#_ENREF_328)three in *Science*,[160](#_ENREF_160), [184](#_ENREF_184), [272](#_ENREF_272) two in *Nature,*[271](#_ENREF_271), [344](#_ENREF_344) two in *Angewandte Chemie International Edition*,[199](#_ENREF_199), [346](#_ENREF_346) 13 in *JACS*,[20](#_ENREF_20), [24](#_ENREF_24), [26](#_ENREF_26), [36](#_ENREF_36), [59](#_ENREF_59), [71](#_ENREF_71), [84](#_ENREF_84), [112](#_ENREF_112), [136](#_ENREF_136), [169](#_ENREF_169), [289](#_ENREF_289), [315](#_ENREF_315), [336](#_ENREF_336) and three in *PNAS*.[5](#_ENREF_5), [148](#_ENREF_148), [318](#_ENREF_318) We published 44 publications during the first MRI grant period,[2-45](#_ENREF_2) 50 publications during the second MRI grant period,[47-96](#_ENREF_47) 62 publications during the third MRI grant period,[97-158](#_ENREF_97) 79 publications during the fourth grant period,[159-237](#_ENREF_159) and 126 peer-reviewed products during this fifth grant period.[238-363](#_ENREF_238) Clearly the impact of undergraduate researchers working with motivated and skilled faculty for the advancement of scientific knowledge is highly significant.

*Transformational Outcomes (Broader Impacts)*

From 2001, when the first NSF-MRI grant was funded, through the summer of 2019, the MERCURY investigators worked with 888 students on research projects. Without double counting female students of color, 75% of our undergraduate research students have been female or male students of color. Approximately half of our graduates attend graduate school for the purpose of obtaining advanced degrees in STEM fields and approximately 2/3 are female and/or students of color. Since the start of the MERCURY consortium students mentored by MERCURY faculty have won more than 50 national awards, including a Rhodes, 10 Fulbright Fellowships, 21 Goldwater Fellowships, two Gates Cambridge Scholarships, and more than 20 national graduate fellowships (NIH, NASA, NDSEG, NSF). We have had more than 1600 attendees at the 18 MERCURY conferences and we have had 111 speakers, 61 of whom have been female and/or faculty of color.

In terms of operations and maintenance, we have had no major downtime and usage history reveals that all of the MERCURY investigators have had adequate computer time on the various HPC clusters we have obtained from MRI funds. PI Shields has invited new investigators into the consortium when others leave in order to optimize the use of these clusters. We have demonstrated we know how to maximize the investment NSF has made in us.

1. **Overview of Past and Current Makeup of Faculty in the MERCURY Consortium**

Since 2016 the resources of the **M**olecular **E**ducation and **R**esearch **C**onsortium in **U**ndergraduate computational chemist**RY** (**MERCURY**) were primarily used by 27 researchers and their undergraduate students: **Anderson,** **Ball**, **Baker**, **Barnes**, **Bhattacharyay**, **Bruce**, **Cafiero**, **Donald**, **Dong**, **Gomez**, **He**, **Kosenkov**, **McDonald**, **Miller**, **Nagan**, **Navea**, **Padgett**, **Parish**, **Patterson**, **Phillips**, S**chrier**, **Shepherd**, **Shields**, **Sumner**, **Tomlinson,** **Van Wynsberghe** and **Varner**. These 27 research groups kept the clusters fully occupied, and we used local and national resources as needed (NSF XSEDE & DOE NERSC). **Dong** has left the consortium, and we added 12 new faculty at the end of 2019, eight at the assistant professor level and four at a senior level. This brings the consortium to 38 researchers at 33 institutions.

Involvement in a highly mentored, exciting undergraduate research project is the key to cultivating and retaining student interest in the sciences and is therefore an excellent means for increasing the diversity of the chemistry community. It has been conclusively demonstrated that active learning has an outsized impact on retaining female students and students of color in STEM fields,[366](#_ENREF_366) and a highly mentored original research project where the student is in charge of their own project is the ultimate active learning experience for all students.[365](#_ENREF_365), [367-368](#_ENREF_367) The three senior faculty who formed the MERCURY consortium in 2000 are **Maria Gomez** (*Mount Holyoke*, materials), **Carol Parish** (*University of Richmond*, physical organic), and **George Shields** (*Furman*, physical). The 12 faculty who joined in the second, third, fourth, and fifth grant proposals, and remain in MERCURY, are **Kelly Anderson** (*Roanoke College*, physical), **Joseph Baker** (*The College of New Jersey*, biochemistry), **Aurelia Ball** (*Skidmore College*, biochemistry), **George Barnes** (*Siena*, physical), **Sudeep Bhattacharyay** (*U. Wisconsin-Eau Clare*, physical biochemistry), **Chrystal Bruce** (*John Carroll*, physical), **Mauricio Cafiero** (*Rhodes*, biochemistry), **Kelling Donald** (*Richmond*, chemical bonding), **Kedan He** (*Eastern Connecticut State University*, biological), **Heidi Hendrickson** (*Lafayette College*, Physical), **Dmitri Kosenkov** (*Monmouth*, physical), **Ashley McDonald** (*Cal Poly*, biophysical), **Bill Miller III** (*Truman State*, biochemistry), **Maria Nagan** (*Truman State*, biochemistry), **Juan Navea** (*Skidmore*, physical), **Eric Patterson** (*Truman State*, physical organic), **Jim Phillips** (*U. Wisconsin-Eau Clare*, physical), **Joshua Schrier** (*Fordham*, Physical), **Tricia Shepherd** (*Westminster*, physical), **Isaiah Sumner** (*James Madison*, biochemistry), **Aimée Tomlinson** (*North Georgia College*, physical), **Mychel Varner** (*Iona,* physical), and **Adam Van Wynsberghe** (*Hamilton*, biochemistry). **Nagan** and **Patterson** moved to SUNY Stony Brook as lecturers; they both run productive undergraduate research groups. **Shepherd** has moved to Franklin & Marshall College.

The 12 additional investigators who joined this academic year are: **Sarah Arradondo** (*Washington),* **Rob Berger** (*Western Washington*), **Clyde Daly** & **Casey Londergan** (*Haverford*), **Wallace Derricotte** (*Morehouse*), **Jay Foley** (*William Paterson)*, **Lindsey Madison** (*Colby*), **Caitlin Scott** (*Hendrix)*, **Patricia Soto** (*Creighton*), **Tyler Luchko** (*Cal State Northridge*), **Simbarashe Nkomo** (*Oxford College*), and **Anton Oliynyk** (*Manhattan*), bringing the total number of participants to 38 faculty at 33 different institutions. **Londergan** is Professor and Chair of his department, while **Berger**, **Soto**, and **Luchko** are Associate Professors, and the other eight are assistant professors. **Scott** is a MERCURY alumna (**Gomez** lab), who joins **Miller** and **Varner** as alumni of MERCURY faculty (**Nagan** & **Parish** labs), and all three attended MERCURY conferences and used MERCURY resources as undergraduates.

The 38 MERCURY investigators now includes 11 full Professors, 10 Associate Professors, 15 Assistant Professors, and two lecturers (formerly full Professors). We know from experience that this balance will allow for effective mentoring across the consortium. The success of MERCURY members is in large part due to the network and support of the group.[1](#_ENREF_1) As the consortium has grown, we have formalized the mentoring process to ensure that each member has a small network to which they belong in addition to the being supported by the larger consortium. The 12 new members will be assigned to a mentoring group to provide access to the knowledge and strategies of established members and allow a seamless transition into the consortium. Activities for mentoring groups include monthly web meetings, writing groups, pre-submission review of manuscripts and grant proposals, and in-person meetings at conferences. Strategies for improving and balancing teaching, research, and service obligations have been particularly helpful to new faculty. The consortium in general and mentoring groups in particular ameliorate the isolation many computational chemists at PUIs feel. Mentoring networks have been shown to improve career success at all stages of an academic career[369](#_ENREF_369) and are an important contributor to the career satisfaction and productivity of MERCURY consortium members. **Chrystal Bruce**, who is a co-PI on two relevant grants from NSF and the Department of Education totaling $2,293,515 [Advancing STEM Careers by Empowering Network Development (ASCEND); Linked Learning and Early Warning Approach for At Risk Student Success (LLASS)] is responsible for managing and assessing the value of our mentoring groups.

Undergraduate research is the key to cultivating and retaining student interest in chemistry and we offer as many of these research opportunities as possible to first and second year students.[370-371](#_ENREF_370) MERCURY faculty are well-funded to support student stipends, with 17 NSF, 2 NIH, 4 ACS/PRF, 2 Dreyfus, 1 Jeffress Foundation, and 3 Research Corporation grants as PIs to support research ($6.37M) as well as three other grants as co-PIs or senior personnel (SP) for research projects ($3.51M). In addition, **Schrier** is the PI of a DARPA grant worth $7.2M and **Bruce** is the PI of a DOE grant worth $650,000. All told, as of the 2019-20 academic year, 22 of the 38 MERCURY faculty hold 41 grants as PIs, worth $14.57M, and are co-PIs/SP on another $3.51M. We expect that the mentoring aspects we’ve developed over the years will greatly enhance the productivity of our newest members, as it has for others. And the addition of computing resources will enhance our undergraduate research programs. The pictures of the 38 MERCURY faculty are shown below.

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| --- | --- | --- | --- | --- |
|  |  |  |  |  |
| Anderson | Arradondo | Baker | Ball | Barnes |
| Sudeep Bhattacharyay |  |  |  |  |
| Bhattacharyay | Berger | Bruce | Cafiero | Daly |
|  | Dr. Kelling J. Donald |  | https://www.mtholyoke.edu/sites/default/files/styles/department_people_page_image/public/acad/chemistry/images/maria-gomez.jpg?itok=5uBZV15I&c=5ff27d7b33911ed6b6f1c036b5f5025e | Kedan He |
| Derricotte | Donald | Foley | Gomez | He |
| d |  |  |  |  |
| Hendrickson | Kosenkov | Londergan | Luchko | Madison |
|  |  |  |  |  |
| Miller | Nagan | Navea | Nkomo | Oliynyk |
| Dr. Carol  Parish |  |  | https://content-calpoly-edu.s3.amazonaws.com/chemistry/1/images/faculty/mcdonald2.jpg |  |
| Parish | Patterson | Phillips | Ringer McDonald | Schrier |
|  | Image result for tricia shepherd | George C. Shields | Patricia Soto Becerra, BA, PhD | https://www.jmu.edu/_images/chemistry/Sumner2-profile.jpg |
| Scott | Shepherd | Shields | Soto | Sumner |
| Image result for aimee tomlinson ung |  |  |  |  |
| Tomlinson | Van Wynsberghe | Varner |  |  |

1. **Overview of MERCURY Faculty Research Efforts**

The MERCURY faculty’s research efforts are summarized briefly below, starting with the faculty who have been in the consortium the longest, and proceeding to our newest members.

**Maria Gomez Research:** The **Gomez group** focuses on charged defect conduction paths with applications to fuel cells. Her earlier work[132-133](#_ENREF_132), [167](#_ENREF_167), [187](#_ENREF_187), [236](#_ENREF_236) showed that there are many possible proton pathways contributing to overall conduction in doped perovskites. Her group showed that, in BaDxZr1-xO3-y  perovskites, an oxygen vacancy[372](#_ENREF_372) near an Al dopant increases the barrier for proton escape from the dopant due to lattice rearrangement while one near Sc and Y dopant decreases the barrier for proton escape from the dopant suggesting that the oxygen vacancy can increase proton conduction in some cases. They are exploring how long-range proton conduction pathways change due to local structure distortions induced by oxygen vacancies and proton/oxygen vacancy correlation, using extensions of their earlier path searching techniques[132](#_ENREF_132), [167](#_ENREF_167), [187](#_ENREF_187), [236](#_ENREF_236), [372](#_ENREF_372) along with dynamical methods,[373-374](#_ENREF_373) to quantify the effect of a delocalized oxygen vacancy on oxygen vacancy conduction.

**Carol Parish's Research:** Research in the **Parish** group employs the tools of quantum mechanics, conformational searching and molecular dynamics simulation to answer questions about the structure, energy, reactivity and/or dynamics of motor proteins, polymerases, damaged DNA, petroleum combustion intermediates, neurosteroids and ion-gated membrane receptors.[13](#_ENREF_13), [15](#_ENREF_15), [17](#_ENREF_17), [58-59](#_ENREF_58), [126-127](#_ENREF_126), [169](#_ENREF_169), [217-218](#_ENREF_217), [220](#_ENREF_220) Current projects include 1.) performing highly correlated, multireference quantum chemical calculations on diradical intermediates found in petroleum combustion, and in formation of anti-cancer warhead drugs and fullerene nanoparticles, 2.) using highly efficient sampling techniques to study the dynamics of HIV-1 protease flap motions and ionotropic glutamate (iGluR) receptor behavior, and 3.) designing novel polyoligomericsilsesquioxane ligands for HIV protease to understand host-guest interactions between iGluR proteins and endogenous ligands. These projects are computationally very demanding, and depend on the availability of fast compute cycles with high speed interconnects.

**George Shields Research:** The **Shields** group has published a series of papers on accurate relative and absolute calculations of pKa values, including careful examination of the best theoretical and experimental values for the free energy of hydration of fundamental ions, and the optimum computational procedures for determining deprotonation equilibrium constants in aqueous solution.[19-20](#_ENREF_19), [23-24](#_ENREF_23), [129](#_ENREF_129), [179](#_ENREF_179) An outgrowth of the groups interest in biochemistry[69](#_ENREF_69), [71](#_ENREF_71), [101](#_ENREF_101), [107-109](#_ENREF_107), [200](#_ENREF_200), [375-378](#_ENREF_375) is understanding the structure of water,[25-26](#_ENREF_25), [379-381](#_ENREF_379) leading to accurate calculations of gas phase water clusters,[28](#_ENREF_28), [60](#_ENREF_60), [67](#_ENREF_67), [102](#_ENREF_102), [131](#_ENREF_131), [143-144](#_ENREF_143), [160](#_ENREF_160), [178](#_ENREF_178), [199](#_ENREF_199), [223](#_ENREF_223), [272](#_ENREF_272) which led to research that focuses on modeling the formation of atmospheric aerosols.[287](#_ENREF_287), [293](#_ENREF_293), [326](#_ENREF_326), [349](#_ENREF_349) Understanding this process will yield information about the initial growth of atmospheric aerosols, and address the large uncertainty associated with the role of aerosols in global warming.[70](#_ENREF_70), [100](#_ENREF_100), [130](#_ENREF_130), [159](#_ENREF_159), [161-162](#_ENREF_161), [198](#_ENREF_198), [327](#_ENREF_327)

**Mauricio Cafiero Research:** The **Cafiero** group studies the binding of small molecules to proteins and the confirmations of small peptides. They investigate acetaminophen metabolism by a sulfotransferase enzyme (SULT1A3),[197](#_ENREF_197) using an active site model from a crystal structure[382](#_ENREF_382) using DFT and MP2 methods. Working with an experimental collaborator, they expanded this study to how a suite of catecholaminic and catecholic molecules interacts with SULT1A3,[228-229](#_ENREF_228) SULT1A1, catechol-o-methyltransferase,[260](#_ENREF_260) phenylalanine hydroxylase,[354](#_ENREF_354) tyrosine hydroxylase,[308](#_ENREF_308) and other enzymes/receptors. They are also working on discovery of inhibitors for the LpxC enzyme for gram-negative bacteria.[285](#_ENREF_285), [305](#_ENREF_305), [383-384](#_ENREF_383)

**Kelling Donald's Research:** In the **Donald** research group, work is focused on (i) halogen bonding and other sigma hole interactions in organic and inorganic systems,[210](#_ENREF_210), [278](#_ENREF_278) (ii) fluxionality in planar inorganic clusters and the nature and potential control of so-called molecular machines,[208](#_ENREF_208), [263](#_ENREF_263) (iii) the evolution of structural preferences and thermal stability in metal halide and hydride molecules, clusters, and corresponding extended solids,[322](#_ENREF_322)(iv) the stability, and catalytic applications of structurally interesting or unusual main group and transition metal organometallic compounds,[151](#_ENREF_151), [231](#_ENREF_231), [351](#_ENREF_351), [385](#_ENREF_385) (v) the stabilization of unusual bonding arrangements, including planar tetra-coordinate and other unusual coordination environments,[172](#_ENREF_172) (vi) quantifying currently qualitative but transferrable concepts in chemical bonding,[233](#_ENREF_233) and (vii) aromaticity and analogous phenomena in non-hydrocarbon systems.[338](#_ENREF_338), [386](#_ENREF_386) The MRI resources are essential for calculations on large and heavy elemental systems.

**Maria Nagan Research:** The **Nagan** group models RNA to understand how chemical functional groups affect structure and biological function.In addition to the standard bases in RNA, there are naturally occurring, post-transcriptionally modified bases. MD studies of human tRNALys,3 found that the *N6*-threonyl-moiety at position 37 is required for maintenance of the anticodon stair-stepped conformation required for correct codon recognition,[56](#_ENREF_56)and systematic natural bond orbital analysis revealed that strong electrostatic interactions between the backbone and the 34th base are key to retaining the structure.[185](#_ENREF_185) A better force field for nonstandard bases is being developed to match experimental sugar pucker ratios.

**Eric Patterson Research:** The **Patterson** group explores issues of environmental chemistry via quantum chemical modeling, including the chemistry of steroids that are common contaminants in surface and wastewater. Working with our collaborators at Iowa State, we have recently established that trenbolone, a bovine growth hormone, completes an unexpected photochemical hydration/thermal dehydration cycle that prolongs its presence in surface waters.[184](#_ENREF_184)

**Tricia Shepherd’s Research:** The **Shepherd** group is studying the transport of water and ions in confined environments because it is central to understanding protein channels in biological systems and material applications involving nanomembrane technology. They plan to build on their success incorporating the monoatomic water (mW) model[387](#_ENREF_387) and complementary coarse-grained interactions including ions[388](#_ENREF_388) and carbon-based nanoparticles.[166](#_ENREF_166), [237](#_ENREF_237), [389](#_ENREF_389) They will extend their analysis to study interactions between water and ions under confinement at the hydrophobic nanopore surface.

**Adam Van Wynsberghe’s Research:** The **Van Wynsberghe** lab is investigating the kinetics and pathways of ligand association to the influenza viral protein neuraminidase (NA).[136](#_ENREF_136) His group has developed a multi-scale methodology to describe the complete binding trajectories of small molecules binding to either the active or secondary site of NA, by first using Brownian Dynamics to compute the distal diffusional approach, and then transitioning to equilibrium MD once the ligand and the protein become proximal, which captures the association dynamics over multiple time scales, followed by post-processing MD trajectories using MM/GBSA to provide insight into the favored pathways of binding. To achieve adequate sampling, they carry out thousands of 5 ns trajectories for this system.

**Kelly Anderson’s** **Research**: The **Anderson** lab uses Monte Carlo molecular simulation techniques to study a variety of complex chemical systems. Currently, their attention is on the interactions of multicomponent liquid solutions with solid substrates.[201](#_ENREF_201) Additional work has focused on mixtures of alkanes with other organic species (alkenes, alcohols, perfluoroalkanes).

**Sudeep Bhattacharyay’s Research**: The **Bhattacharyay** lab group studies the chemistry of enzymes, such as the role of dynamics and quantum mechanical tunneling in a flavin-containing enzyme.[390-391](#_ENREF_390) Using extensive MD simulations, they are developing a molecular model of the interplay of dynamics and quantum tunneling in enzyme catalysis,[290](#_ENREF_290), [391](#_ENREF_391) and exploring the role of macromolecular crowding on conformational dynamics and enzyme catalysis of bacterial prolyl-tRNA synthetase.[174](#_ENREF_174), [195](#_ENREF_195), [204-205](#_ENREF_204), [332](#_ENREF_332)

**James Phillips Research:** The **Phillips** group studies condensed-phase effects on the structural properties of molecular complexes; primarily electron donor-acceptor systems (*e.g.*, CH3CN–BF3),[392-393](#_ENREF_392) and hydrogen-bonded/proton-transfer systems.[273](#_ENREF_273) Using low-temperature IR spectroscopy, they assess the extent of structural change across various media via measured frequency shifts. Computations are vital for characterizing gas-phase systems and providing direct insight into the mechanism for medium-induced structural change[181](#_ENREF_181), [213](#_ENREF_213), [393](#_ENREF_393) and enable them to identify promising targets and focus their experimental efforts.[181](#_ENREF_181), [394-395](#_ENREF_394) Following up on their initial work on Group IV halides (MX4: M = Ti, Si, Ge; X=F,Cl),[211](#_ENREF_211), [298](#_ENREF_298), [310](#_ENREF_310) they are exploring the nitrile and imine complexes of the monoalkyl analogs (MX3R) of these acids.

**Aimée Tomlinson Research:** The **Tomlinson** group researches how the electronic, optical, and structural properties of conjugated oligomer materials vary as a function of conjugation. Using a combination of organic synthesis, theoretical calculations & physical measurements they carry out systematic investigations of novel cross-conjugated oligomers based on the benzo[1,2-*d*;4,5-*d’*]bisoxazole (BBO) moiety. This unique electron-deficient ring system with two distinct conjugation axes: 2,6-conjugation through the oxazole rings, and 4,8-conjugation through the central benzene ring, and spatially segregated frontier molecular orbitals (FMO)s, provides a platform for tuning of the LUMO or HOMO by varying the nature of the substituents and their arrangement around the central molecule.[163-164](#_ENREF_163), [192](#_ENREF_192), [207](#_ENREF_207), [396-397](#_ENREF_396)

**George Barnes Research:** The **Barnes** group studies the reaction dynamics that take place in tandem mass spectrometry systems, in particular, MS2 techniques for proteomic analysis which involve the initial separation of an ion of interest (MS step 1), which is then highly energized and dissociates. The dissociation products are then mass analyzed (MS step 2), which leads to sequencing information. However, the presence of post-translational modifications (PTMs) of peptides, such as methylation, acetylation, phosphorylation, sulfonation, and disulfide bonding, can greatly complicate the identification of the peptide sequence. PTM is a common occurrence in biological systems, and can occur at the N- or C-terminus as well as the side chain of an amino acid. It has been estimated that between 40%-70% of MS2 spectra cannot be matched or are misidentified.[398](#_ENREF_398) Because of its utility, there is significant interest in understanding the chemical and physical characteristics of MS2 systems.[399-407](#_ENREF_399) The Barnes group has studied surface induced dissociation (SID) of protonated peptides colliding with organic self-assembled monolayer (SAM) surfaces[408-410](#_ENREF_408) as well as reactive landing (RL) of protonated peptides on modified SAM surfaces,[411](#_ENREF_411) which has demonstrated the importance of proton mobility and non-covalent interactions.

**Chrystal Bruce Research:** The **Bruce** lab focuses on understanding the molecular-level interactions that exist between biologically relevant molecules, specifically small molecule DNA minor groove binders and protein/ligand interactions. Retinoic acid (RA), a form of vitamin A, was originally predicted to reduce the spread of cancer. But in some cases cancer cell growth is actually promoted by the introduction of retinoic acid *in vivo* in rats.[412](#_ENREF_412) This observation was explained by the concentration ratios of two proteins in the specific cell type (FAPB5 and CRABPII). When RA binds to FABP5, a survival pathway is created in the cancerous cells and results in cell proliferation. When in the presence of CRABPII, RA is carried to retinoic acid receptors (RAR), which lead to apoptosis and the inhibition of tumor growth. The Bruce group has published the first MD study showing the structure and dynamics of these systems,[312](#_ENREF_312) and are studying small molecules that may promote the natural apoptotic process when bound to FABP5.

**Dmitri Kosenkov Research:** The **Kosenkov** lab is studying fundamental interactions of electronic excited states of organic chromophores used as molecular sensors (e.g. pyridinium *N*-phenolate betaine dyes and boron-dipyrromethene) in organic solvents to obtain detailed atomistic-level knowledge of mechanisms of energy transfer,[413](#_ENREF_413) and continue to enhance their expertise in modeling intermolecular interactions,[414-416](#_ENREF_414) fragmentation EFP and FMO methods,[234](#_ENREF_234), [417-418](#_ENREF_417) and hybrid QM/MM methodologies that interface electronic structure methods for electronic excited states with EFP.[419](#_ENREF_419)

**Ashley Ringer McDonald Research:** The **McDonald** group studies molecular interactions in complex macromolecular systems using correlated electronic structure techniques and molecular simulations to computationally characterize ligand/aptamer binding to understand the structural and energetic changes that occur in molecular recognition events involving DNA and RNA aptamers. They are also developing a computational model of MEK1, a key protein involved in the RAF-MEK-ERK cascade, which is activated in many tumor cell lines and in the tumors of cancer patients,[356](#_ENREF_356) which they will use to screen small molecule inhibitors of MEK1. This project is not feasible without the MERCURY resources.

**Bill Miller III Research:** The **Miller** group studies problems in biochemistry using MD, including studies on DNA binding proteins.[218](#_ENREF_218), [220](#_ENREF_220), [274](#_ENREF_274), [294-295](#_ENREF_294), [299](#_ENREF_299), [303](#_ENREF_303), [329](#_ENREF_329), [331](#_ENREF_331), [352](#_ENREF_352) Current work includes designing an isoflavanone derivative for aromatase inhibition to treat endometriosis, and inhibiting the aggregation of amyloid beta proteins found in the brains of patients with Alzheimer’s Disease (AD). Specifically, they are studying a class of molecules called polyphenols that have shown promising experimental results for AD.

**Juan Navea Research:** The **Navea** group investigates problems in physical chemistry of interfaces. This includes how tropospheric gases bind onto atmospheric aerosols, leading to various coordination modes between surface (aerosol) and substrate (adsorbed trace gases).[420-424](#_ENREF_420) Among the components of aerosols are semiconductor compounds, such as TiO2, that can trigger photo-induced heterogeneous reactions on the substrate.[425-427](#_ENREF_425) They are modeling the nitrate-TiO2 interface using computational chemistry methods. In addition, they investigate the substrate’s vibrational frequency shifts resulting from the co-adsorption of water and nitrates on TiO2 active sites.[428-430](#_ENREF_428) Modeling the aerosol interaction with trace atmospheric gases will add to our understanding of the indirect effects of atmospheric aerosols on climate change.Moving from computational studies using PC workstations to the MERCURY resources has been essential to increase the computational efficiency of our surface-substrate models.

**Joshua Schrier Research**: The **Schrier** group uses simulations and machine learning to understand and design organic-inorganic hybrid materials for energy and environmental problems. In particular they are interested in understanding the role of non-covalent interactions in controlling inorganic topologies,[343](#_ENREF_343) the role of reaction conditions and reagent properties on reaction outcome,[330](#_ENREF_330) and how human biases in experimental decision making hinder progress in machine learning using those datasets.[344](#_ENREF_344) Current computational will contribute to understanding molecular interactions in the formation of precursor solutions and electrolyte solution properties.

**Isaiah Sumner Research:** The **Sumner** group uses classical MD, *ab initio* molecular dynamics (AIMD) and electronic structure theory to study enzyme mechanisms. The transfer of an acetyl group or ubiquitin to a target protein are two examples of a process called protein post-translational modification (PTM), which allows cells to rapidly respond to internal and external stimuli. Despite the importance of acetyl and ubiquitin transferases,[431-432](#_ENREF_431) there are currently no studies that conclusively show the enzymes’ reaction pathways.[433-435](#_ENREF_433) The group aims to determine and compare the reaction pathways for representative members of the acetyl and ubiquitin transfer family of enzymes using AIMD and QM/MM electronic structure calculations.[301](#_ENREF_301), [345](#_ENREF_345) MERCURY resources are crucial to the success of this project.

**Mychel Varner Research:** The current research of the **Varner** group concerns reactions of neonicotinoid insecticides with atmospheric species and a collaboration with a synthetic organic chemist, requiring high-level ab initio calculations on small complexes. They also investigate new particle formation (NPF) in the atmosphere,[436-437](#_ENREF_436) and have shown that although amines typically have concentrations 1–3 orders of magnitude lower than that of NH3 in the atmosphere, they still play an important role in driving NPF.[255](#_ENREF_255)

**Sarah Arradondo Research**: The **Arradondo** lab characterizes various non-covalent interactions within interesting systems using *ab initio* methods and density functionals in conjugation with large, robust basis sets.[438-441](#_ENREF_438) They are currently investigating the different configurations within several room temperature ionic liquids along with the hydrogen bond networks that these materials have with water and how these interactions may affect the materials bulk phase properties when including a co-solvent.

**Joseph Baker Research:** The **Baker** group uses molecular dynamics simulations to investigate the biomechanical properties of type IV pilus (T4P) filaments and the interactions of ionic liquid/deep eutectic solvents with proteins and membranes. They use a comprehensive, multi-scale computational approach, including both all-atom and coarse-grained molecular dynamics simulations, to characterize the T4P structural ensemble, identify the most important inter-monomer interactions for T4P stability and strength, and develop a coarse-grained model to accurately describe the force-transitioned state of a T4P filament.[442-443](#_ENREF_442)We also investigate the influence of ionic liquids and deep eutectic solvents on the conformation of proteins and small peptides including Trp-cage and insulin,[281](#_ENREF_281), [444](#_ENREF_444)and also how these solvents embed in the lipid bilayer[340](#_ENREF_340) and impact the permeability of lipid bilayers to small molecules.

**Aurelia Ball Research:** The **Ball** group aims to understand how intrinsically disordered proteins interact with and influence more structured proteins in order to perform their function as part of different cellular and disease processes,[251](#_ENREF_251) including studying how the disordered HIV protein Vif interacts with human proteins to protect the virus from antiviral defenses,[333](#_ENREF_333) and characterizing the binding pathway for a proline-rich disordered peptide that binds an SH3 domain to pass information in cellular signaling.

**Robert Berger Research:** The **Berger** group uses DFT to study relationships between the structure and properties of crystalline materials, primarily for solar energy conversion. Most projects focus on predicting and understanding the effects of structural tunability (via doping, substitution, temperature-controlled distortions, and/or strain) on the electronic band structure and band gap of light-absorbing perovskite compounds. These perovskites include both halide photovoltaics (e.g., CH3NH3PbI3)[445](#_ENREF_445) and oxide photocatalysts (e.g., SrTiO3).[446-447](#_ENREF_446) They use the VASP code and MERCURY resources will facilitate the computation of larger-unit-celled structures (e.g., layered and/or doped perovskite superstructures).

**Clyde Daly Research:** The **Daly** research group will use computations of vibrational spectroscopy to investigate the dynamics & structure of complex condensed phase systems,[448-454](#_ENREF_448) and use non-equilibrium MD to investigate nanomaterials. Specific projects include: (1) using machine learning techniques to build more accurate maps between QM calculations of vibrational frequencies for single reporters and classical simulations of their condensed phase dynamics, (2) simulating the spectroscopy of CO2 and water in mixtures of ionic liquids,[448-449](#_ENREF_448), [451](#_ENREF_451), [453](#_ENREF_453) (3) describing the sequestration behavior of acyl carrier proteins using Raman spectroscopy of attached alkyl probes,[450](#_ENREF_450) and (4) determining the interaction between biomolecules and nanomaterials using non-equilibrium MD simulations. These projects require a wide range of computing resources and software, so the MERCURY resources are essential.

**Wallace Derricotte Research**: The **Derricotte** group focuses on studying the effect of noncovalent interactions on reaction mechanisms, with a new method that involves decomposing the reaction force using symmetry-adapted perturbation theory (SAPT).[455](#_ENREF_455) They have developed a free open-source Python package, PYREX (PYthon Reaction Energy eXtension), that implements their SAPT reaction force method and numerous other techniques that provide novel insight into the chemical and physical driving forces of chemical reactions (<https://github.com/WDerricotte/pyrex>). They are investigating a series of antioxidant molecules to quantify the effect of noncovalent interactions between the antioxidant and various reactive oxygen species. This project absolutely requires the MERCURY computing resources.

**Jonathan Foley Research**: The **Foley** lab leverages multi-scale theoretical and computational approaches, bridging quantum mechanical and electrodynamics methods, to study fundamental aspects of light-matter interactions and to enable the design of materials to control light, heat, and chemical reactivity. Key scientific outcomes so far include the discovery of an emergent optical phenomenon in composite nanoparticles known as “scattering mediated absorption”,[456-458](#_ENREF_456) and the development of an open-source software package, [WPTherml](https://foleylab.github.io/wptherml/), for designing materials for harnessing heat.[459-460](#_ENREF_459)

**Kedan He Research**: The **He** group is expert on electronic structure methods,[461](#_ENREF_461) and is currently developing machine learning algorithms for fast mining to extrapolate meaningful information from databases of chemical structures to discover and design molecules with important biological properties, such as (1) ligand & structure-based virtual screening to discover novel EGFR inhibitors and (2) virtual screening and identification of potential illegal synthetic cathinones.

**Heidi Hendrickson Research:** The **Hendrickson** lab uses computational methods to (1) utilize and develop multiscale computational approaches (DFT, QM/MM, MD) to model charge transfer and transport properties in semiconducting polymeric materials,[277](#_ENREF_277) (2) utilize computational methods (protein-ligand docking, QM/MM, MD, protein network analysis) to identify and characterize protein-ligand interactions in G-protein coupled receptors,[318](#_ENREF_318) and (3) utilize electronic structure calculations to characterize highly-absorbing species in atmospheric brown carbon aerosols.[339](#_ENREF_339)

**Casey Londergan Research**: The **Londergan** group uses all-atom simulations of proteins with artificial “vibrational probe” functional groups to better understand the experimental data associated with IR and Raman spectra of those probe groups. They conduct well-sampled MD simulations in explicit solvent to understand the protein’s overall conformational distribution, then they include the probe groups explicitly and use fragment-potential-based frequency calculations[462](#_ENREF_462) to directly simulate the spectra.

**Tyler Luchko Research**: The **Luchko** lab uses computational methods to study the solvation of small molecules and biomolecules at the molecular scale, and they are actively developing the 3D reference interaction site model (3D-RISM) of molecular solvation,[463](#_ENREF_463) which uses statistical physics to predict the molecular distribution of explicit, all-atom solvent models around solute molecules and calculate the solvation thermodynamics from these distributions.[464](#_ENREF_464) Using 3D-RISM, they can predict properties of the solute molecules, such as solvation free-energy, enthalpy and entropy,[465](#_ENREF_465) hydrophobicity,[466](#_ENREF_466) protein-drug binding affinities,[467](#_ENREF_467) and the distribution of water and ions around solutes.[468-471](#_ENREF_468)

**Lindsey Madison Research**: The **Madison** group studies vibrational motions of clathrate hydrates, a naturally forming, crystalline phase of water characterized by the presence of non-polar, small molecules such as carbon dioxide or methane.[472-473](#_ENREF_472) Better understanding of this material can advance knowledge about the role clathrate hydrates play in global climate change,[474](#_ENREF_474) the unintentional and disastrous formation in pipelines,[475-476](#_ENREF_475) and their relevance in astrochemical reactions.[477](#_ENREF_477) More fundamentally, clathrate hydrates are a unique host-guest system because the relatively weak intermolecular forces that hold the lattice together result in an extremely flexible host.[478-480](#_ENREF_478) We study the vibrational wave function of these materials to predict the complete vibrational spectrum and compare them to classical MD simulations,[480-481](#_ENREF_480) as well as electronic structure calculations of small and medium sized clusters.[482-485](#_ENREF_482)

**Simbarashe Nkomo Research**. The **Nkomo** research group[486-489](#_ENREF_486) working in collaboration with an experimental organic synthesis group, uses computational methods to study stability properties of cyclobutadiene derivatives, and uses the information to propose synthetic routes for highly conjugated target molecules such as 10,11diphenylcyclobuta[5,6]pyrazino[2,3f][1,10]phenanthroline.

**Anton Oliynyk Research**: The **Oliynyk** group studies intermetallic compounds and combines machine-learning methods with experimental research.[490-495](#_ENREF_490) They study the inorganic chemistry of intermetallics materials with focus on energy converting materials and mechanical properties, such as hardness and wear resistance.[493](#_ENREF_493) The materials are synthesized directly from elements by high-temperature methods, including arc-melting and sintering methods. A cutting-edge machine-learning-driven approach[492](#_ENREF_492) is utilized to guide the discoveries of novel materials and screen chemical space for potential compounds, and computational methods are used for structure prediction from first principles.

**Caitlin Scott Research:** The **Scott** lab[496-501](#_ENREF_496) uses computational tools to predict the structures of G protein-coupled receptors (GPCRs) at various stages of activation for structure-based drug design.[502-504](#_ENREF_502) Approximately one-third of drugs approved by the FDA target this family of proteins.[505](#_ENREF_505) Unfortunately, GPCRs are quite flexible and dynamic, and despite the recent advances in protein crystallography, the conformations of GPCRs at various activation states remain unknown. They will use the MERCURY computational resources to run molecular dynamics (MD) simulations of the proteins in a solvated and neutralized lipid bilayer at room temperature and pressure to simulate the proteins in a realistic cellular environment to determine the stability of protein-drug complexes.

**Patricia Soto Research**: The **Soto** group focuses on deciphering the pathological folding behavior of prion proteins, the main component of the infectious prion agent responsible for prion disorders,[506](#_ENREF_506) using computational biophysics techniques. The conformational conversion of the cellular form of the prion protein PrPC to the misfolded and aggregated isoform PrPSc is the key pathological event in prion diseases.[507](#_ENREF_507) The MERCURY facilities are instrumental to examine the hypothesis that prion protein - RNA molecule interactions modulate the protein dimerization mechanism in a protein sequence-dependent manner. To this goal, we will implement a multi-scale computational protocol that benefits from our demonstrated experience in identifying structural dynamics features of prion protein peptides[508](#_ENREF_508) and prion protein in the bulk.[509](#_ENREF_509)

1. **Conclusions and Educational Impact**

We believe that mentoring students in meaningful research projects is a valuable and integral part of being a research active chemist at an undergraduate institution and we choose careers at PUIs with the intention of focusing our energy on undergraduate student involvement. Our objective upon forming the MERCURY consortium was to help our undergraduate research programs to flourish and this has indeed occurred. To highlight one measure of success, from 2001-2019, we published an average of 1.7 papers/year/faculty, which is 3.4 times greater than the usual productivity of a faculty member at a PUI.[46](#_ENREF_46)From 2001 through the summer of 2019, the MERCURY faculty published 361 peer-reviewed products, including two in *Chemical Society Reviews*, one in *Chemical Reviews*, one in *Nature Reviews Chemistry,* three in *Science*, two in *Nature,* three in *Angewandte Chemie International Edition*, 13 in *JACS*, and three in *PNAS*. We have demonstrated that the MERCURY consortium provides an ideal environment for providing research experiences for undergraduates. We are a productive and synergistic consortium with a diverse group of students and faculty; 2/3 of our students over the past two decades were female or students of color. Every time we expand our consortium we further increase the number of high-quality undergraduate research experiences and enhance diversity in the chemical sciences workforce.

When we started in 2001, our goals were twofold: (1) to acquire a supercomputer that would allow us to train undergraduates in computational chemistry, and (2) allow us to achieve excellent research results. Our diverse research interests required a computational system that would allow us to run quantum and molecular dynamics simulations with a variety of different software. Our students were excited and inspired by participating in cutting-edge research projects, so that many of them matriculated to graduate work, or became citizens with a keener understanding of what research is and how it works. The technical support we hired as part of the first grant was essential for maintaining our shared computer system and assuring we split computer time fairly. We had diversity in mind from the very beginning, both with the selection of the initial faculty in the consortium and in the mindset of the faculty. Our idea was to form a northeastern consortium, where we could easily share ideas at an end of summer conference, and learn and network with scientists at research universities, industry, and government laboratories. After our first grant it dawned on us that we could be national in scope, and as we added resources with subsequent NSF MRI grants we expanded nationally.

We realized that the conference was the single most brilliant initiative we had started, and we found money to support it after the first grant period. From the very beginning we opened the meeting to everyone from any institution, with the stipulation that only undergraduates were to present in the poster session. The mentoring, networking, and inspiration that happens at the annual conferences is a must for our faculty, and faculty who stop attending conferences with their students generally realize it is time to step out of MERCURY. Faculty who we invited to join MERCURY are motivated to have active and diverse research groups, and we ask their deans and provosts to make sure they have funding to attend our meeting. As time went on, **Shields** became better at advising speakers on how to structure their talks for the most benefit to the PUI audience. Our undergraduates moved from just listening in the early days, to listening and asking questions in later conferences. A key component of the meetings success is the undergraduate poster session, where experts are present to talk with students at their posters and with the PUI faculty who attend the meeting, increasing the value of the meeting for everyone in attendance. In addition, the meeting provides a dedicated time for the MERCURY faculty to mentor and advise each other. Students from any one particular research group are always amazed to learn how their own work is put into context and are stimulated by the problems that other groups are trying to solve, as well as their methods for trying to solve them. STEM conferences have historically suffered from a lack of female and faculty of color representation, and our efforts to recruit diverse speakers is another key part of the conference as students have visible role models, both from the invited speakers and from the other PUI faculty in attendance. We have had more than 1600 attendees at the 18 MERCURY conferences, with 111 invited speakers, 61 of whom have been female and/or faculty of color. One of the advantages of NSF funding is that the required annual evaluations focuses the entire MERCURY faculty on student outcomes and research results. Faculty returning from the conference to their home institutions are motivated as they start the next academic year. Overall our main goals have not changed and we have been thrilled with our joint success.

The MERCURY consortium has been an outstanding program that has contributed greatly to the development of scientifically trained undergraduates, with a particular focus on diversity and inclusion.[1](#_ENREF_1) Without double counting female students of color, 75% of our undergraduate research students have been female or male students of color. About half of our alumni attend graduate school to obtain advanced degrees in STEM fields and approximately 2/3 are female and/or students of color. Students mentored by MERCURY faculty have been recognized with more than 50 national awards, including a Rhodes, 10 Fulbright Fellowships, 21 Goldwater Fellowships, two Gates Cambridge Scholarships, and more than 20 national graduate fellowships (NIH, NASA, NDSEG, NSF). For more information, see <https://mercuryconsortium.org>

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**References**

1. Shields, G. C., The Molecular Education and Research Consortium in Undergraduate computational chemistRY (MERCURY): Twenty Years of Exceptional Success Supporting Undergraduate Research and Inclusive Excellence. *Scholarship and Practice of Undergraduate Research* **2019,** *3* (Winter 2019), 5-15.

2. Pratt, L. R.; LaViolette, R. A.; Gomez, M. A.; Gentile, M. E., Quasi-chemical theory for the statistical thermodynamics of the hard-sphere fluid. *J. Phys. Chem. B* **2001,** *105* (47), 11662-11668.

3. Grabowski, P.; Riccardi, D.; Gomez, M. A.; Asthagiri, D.; Pratt, L. R., Quasi-chemical theory and the standard free energy of H+(aq). *J. Phys. Chem. A* **2002,** *106* (40), 9145-9148.

4. Asthagiri, D.; Pratt, L. R.; Kress, J. D.; Gomez, M. A., The hydration state of HO-(aq). *Chemical Physics Letters* **2003,** *380* (5-6), 530-535.

5. Asthagiri, D.; Pratt, L. R.; Kress, J. D.; Gomez, M. A., Hydration and mobility of HO-(aq). *Proc. Natl. Acad. Sci. U. S. A.* **2004,** *101* (19), 7229-7233.

6. Greathouse, J. A.; Bemis, G.; Palaban, R. T., Molecular dynamics simulation of the uranyl ion near quartz surfaces. *Proceedings of the International Symposium on Water-Rock Interaction* **2001,** *1*, 173.

7. Greathouse, J. A.; O'Brien, R. J.; Bemis, G.; Pabalan, R. T., Molecular dynamics study of aqueous uranyl interactions with quartz (010). *J. Phys. Chem. B* **2002,** *106* (7), 1646-1655.

8. Greathouse, J. A.; Storm, E. W., Calcium hydration on montmorillonite clay surfaces studied by Monte Carlo simulation. *Molecular Simulation* **2002,** *28* (6-7), 633-647.

9. Zaidan, O. F.; Greathouse, J. A.; Pabalan, R. T., Computer simulation of uranyl adsorption on montmorillonite clay. *Geochimica Et Cosmochimica Acta* **2002,** *66* (15A), A868-A868.

10. Zaidan, O. F.; Greathouse, J. A.; Pabalan, R. T., Monte Carlo and molecular dynamics simulation of uranyl adsorption on montmorillonite clay. *Clays and Clay Minerals* **2003,** *51* (4), 372-381.

11. Greathouse, J. A.; Cygan, R. T., Molecular dynamics simulation of uranyl(VI) adsorption equilibria onto an external montmorillonite surface. *Phys. Chem. Chem. Phys.* **2005,** *7* (20), 3580-3586.

12. Greathouse, J. A.; Stellalevinsohn, H. R.; Denecke, M. A.; Bauer, A.; Pabalan, R. T., Uranyl surface complexes in a mixed-charge montmorillonite: Monte Carlo computer simulation and polarized XAFS results. *Clays and Clay Minerals* **2005,** *53* (3), 278-286.

13. Parish, C.; Lombardi, R.; Sinclair, K.; Smith, E.; Goldberg, A.; Rappleye, M.; Dure, M., A comparison of the low mode and Monte Carlo conformational search methods. *Journal of Molecular Graphics & Modelling* **2002,** *21* (2), 129-150.

14. Parish, C. A.; Zeldin, M.; Pratt, J., Conformational analysis and modeling studies of synthetic 4-dialkylaminopyridine-siloxane oligomers with selective esterase activity. *Journal of Inorganic and Organometallic Polymers* **2002,** *12* (1-2), 31-47.

15. Castillo, H.; Yarger, M.; Rappleye, M.; Parish, C., A comparison of the AMBER\*, OPLSAA and HF potential energy surfaces for a series of diastereomeric cyclic urea HIV-1 inhibitors. *Theochem-J. Mol. Struct.* **2004,** *710* (1-3), 73-76.

16. Macaluso, M.; Parish, C. A.; Hoffmann, R.; Scott, L. T., Dicyclobuta[de,ij]naphthalene and dicyclopenta[cd,gh]pentalene: A theoretical study. *J. Org. Chem.* **2004,** *69* (23), 8093-8100.

17. Parish, C. A.; Yarger, M.; Sinclair, K.; Dure, M.; Goldberg, A., Comparing the conformational behavior of a series of diastereomeric cyclic urea HIV-1 inhibitors using the Low Mode : Monte Carlo conformational search method. *Journal of Medicinal Chemistry* **2004,** *47* (20), 4838-4850.

18. Feldgus, S.; Shields, G. C., An ONIOM study of the Bergman reaction: a computationally efficient and accurate method for modeling the enediyne anticancer antibiotics. *Chemical Physics Letters* **2001,** *347* (4-6), 505-511.

19. Liptak, M. D.; Shields, G. C., Experimentation with different thermodynamic cycles used for pK(a) calculations on carboxylic acids using complete basis set and gaussian-n models combined with CPCM continuum solvation methods. *International Journal of Quantum Chemistry* **2001,** *85* (6), 727-741.

20. Liptak, M. D.; Shields, G. C., Accurate pK(a) calculations for carboxylic acids using Complete Basis Set and Gaussian-n models combined with CPCM continuum solvation methods. *Journal of the American Chemical Society* **2001,** *123* (30), 7314-7319.

21. Pokon, E. K.; Liptak, M. D.; Feldgus, S.; Shields, G. C., Comparison of CBS-QB3, CBS-APNO, and G3 predictions of gas phase deprotonation data. *J. Phys. Chem. A* **2001,** *105* (45), 10483-10487.

22. Sherer, E. C.; Bono, S. J.; Shields, G. C., Further quantum mechanical evidence that difluorotoluene does not hydrogen bond. *J. Phys. Chem. B* **2001,** *105* (35), 8445-8451.

23. Toth, A. M.; Liptak, M. D.; Phillips, D. L.; Shields, G. C., Accurate relative pK(a) calculations for carboxylic acids using complete basis set and Gaussian-n models combined with continuum solvation methods. *J. Chem. Phys.* **2001,** *114* (10), 4595-4606.

24. Liptak, M. D.; Gross, K. C.; Seybold, P. G.; Feldgus, S.; Shields, G. C., Absolute pK(a) determinations for substituted phenols. *Journal of the American Chemical Society* **2002,** *124* (22), 6421-6427.

25. Dunn, M. E.; Pokon, E. K.; Shields, G. C., The ability of the Gaussian-2, Gaussian-3, Complete Basis Set-QB3, and Complete Basis Set-APNO model chemistries to model the geometries of small water clusters. *International Journal of Quantum Chemistry* **2004,** *100* (6), 1065-1070.

26. Dunn, M. E.; Pokon, E. K.; Shields, G. C., Thermodynamics of forming water clusters at various temperatures and pressures by Gaussian-2, Gaussian-3, Complete Basis Set-QB3, and Complete Basis Set-APNO model chemistries; Implications for atmospheric chemistry. *Journal of the American Chemical Society* **2004,** *126* (8), 2647-2653.

27. Palascak, M. W.; Shields, G. C., Accurate experimental values for the free energies of hydration of H+, OH-, and H3O+. *J. Phys. Chem. A* **2004,** *108* (16), 3692-3694.

28. Day, M. B.; Kirschner, K. N.; Shields, G. C., Pople's Gaussian-3 model chemistry applied to an investigation of (H2O)(8) water clusters. *International Journal of Quantum Chemistry* **2005,** *102* (5), 565-572.

29. Pickard, F. C.; Pokon, E. K.; Liptak, M. D.; Shields, G. C., Comparison of CBS-QB3, CBS-APNO, G2, and G3 thermochemical predictions with experiment for formation of ionic clusters of hydronium and hydroxide ions complexed with water. *J. Chem. Phys.* **2005,** *122*.

30. Stewart, E.; Shields, R. L.; Taylor, R. S., Molecular dynamics simulations of the liquid/vapor interface of aqueous ethanol solutions as a function of concentration. *J. Phys. Chem. B* **2003,** *107* (10), 2333-2343.

31. Taylor, R. S.; Shields, R. L., Molecular-dynamics simulations of the ethanol liquid-vapor interface. *J. Chem. Phys.* **2003,** *119* (23), 12569-12576.

32. Speer, O. F.; Wengerter, B. C.; Taylor, R. S., Molecular dynamics simulations of simple liquids. *Journal of Chemical Education* **2004,** *81* (9), 1330-1332.

33. Cullen, D. L.; Desai, L. V.; Shelnutt, J. A.; Zimmer, M., Conformational analysis of the nonplanar deformations of cobalt porphyrin complexes in the Cambridge structural database. *Structural Chemistry* **2001,** *12* (2), 127-136.

34. Chen, M. C.; Lambert, C. R.; Urgitis, J. D.; Zimmer, M., Photoisomerization of green fluorescent protein and the dimensions of the chromophore cavity. *Chemical Physics* **2001,** *270* (1), 157-164.

35. Warren, A.; Zimmer, M., Computational analysis of Thr203 isomerization in green fluorescent protein. *Journal of Molecular Graphics & Modelling* **2001,** *19* (3-4), 297-303.

36. Donnelly, M.; Fedeles, F.; Wirstam, M.; Siegbahn, P. E.; Zimmer, M., Computational analysis of the autocatalytic posttranslational cyclization observed in histidine ammonia-lyase. A comparison with green fluorescent protein. *Journal of the American Chemical Society* **2001,** *123* (20), 4679-4686.

37. Fedeles, F.; Zimmer, M., Conformational/configurational analysis of all the binding geometries of cobalt(III) bleomycin. *Inorganic Chemistry* **2001,** *40* (7), 1557-1561.

38. Zimmer, M., Molecular mechanics, data and conformational analysis of first-row transition metal complexes in the Cambridge Structural Database. *Coordination Chemistry Reviews* **2001,** *212*, 133-163.

39. Davis, T. V.; Zaveer, M. S.; Zimmer, M., Using the Cambridge Structural Database to introduce important inorganic concepts. *Journal of Chemical Education* **2002,** *79* (10), 1278-1280.

40. Todd, L. N.; Zimmer, M., Moderating influence of proteins on nonplanar tetrapyrrole deformations: Coenzyme F430 in methyl-coenzyme-M reductase. *Inorganic Chemistry* **2002,** *41* (25), 6831-6837.

41. Zimmer, M., Green fluorescent protein (GFP): Applications, structure, and related photophysical behavior. *Chemical Reviews* **2002,** *102* (3), 759-781.

42. Zaveer, M. S.; Zimmer, M., Structural analysis of the immature form of the GFP homologue DsRed. *Bioorganic & Medicinal Chemistry Letters* **2003,** *13* (22), 3919-3922.

43. Baffour-Awuah, N. Y. A.; Zimmer, M., Hula-twisting in green fluorescent protein. *Chemical Physics* **2004,** *303* (1-2), 7-11.

44. De Bari, H.; Zimmer, M., Structural analysis of the conformational flexibility of tris(pyrazolyl)borate ligands and their analogues. *Inorganic Chemistry* **2004,** *43* (11), 3344-3348.

45. Desai, L. V.; Zimmer, M., Substrate selectivity and conformational space available to bromoxynil and acrylonitrile in iron nitrile hydratase. *Dalton Transactions* **2004,** (6), 872-877.

46. *Academic Excellence: The Sourcebook.* Research Corporation: 2001.

47. Gao, D.; Svoronos, P.; Wong, P.; Maddalena, D.; Hwang, J.; Walker, H., pK(a) of acetate in water: A computational study *J. Phys. Chem. A* **2005,** *109* (47), 10776-10785.

48. Glassey, W. V., Energy partitioning studies of adsorbate repulsion: Chemisorption and coadsorption of CO and NO on the Pd(111) surface. *Surface Science* **2006,** *600* (1), 173-194.

49. Glassey, W. V., Spreadsheet modeling of electron distributions in solids. *Journal of Chemical Education* **2006,** *83* (2), 327-333.

50. Gomez, M. A.; Griffin, M. A.; Jindal, S.; Rule, K. D.; Cooper, V. R., The effect of octahedral tilting on proton binding sites and transition states in pseudo-cubic perovskite oxides. *J. Chem. Phys.* **2005,** *123* (9).

51. Gomez, M. A.; Peart, P., Including quantum subsystem character within classical equilibrium simulations. *J. Chem. Phys.* **2006,** *125* (3).

52. Gomez, M. A.; Jindal, S.; Fletcher, K. M.; Foster, L. S.; Addo, N. D. A.; Valentin, D.; Ghenoiu, C.; Hamilton, A., Comparison of proton conduction in KTaO3 and SrZrO3. *J. Chem. Phys.* **2007,** *126* (19).

53. Gomez, M. A.; Pratt, L. R.; Kress, J. D.; Asthagiri, D., Water adsorption and dissociation on BeO(001) and (100) surfaces. *Surface Science* **2007,** *601* (6), 1608-1614.

54. Polaske, N. W.; Wood, A. L.; Campbell, M. R.; Nagan, M. C.; Pollak, L. M., Amylose determination of native high-amylose corn starches by differential scanning calorimetry. *Starch-Starke* **2005,** *57* (3-4), 118-123.

55. Hati, S.; Ziervogel, B.; SternJohn, J.; Wong, F. C.; Nagan, M. C.; Rosen, A. E.; Siliciano, P. G.; Chihade, J. W.; Musier-Forsyth, K., Pre-transfer editing by class II prolyl-tRNA synthetase - Role of aminoacylation active site in "selective release" of noncognate amino acids. *Journal of Biological Chemistry* **2006,** *281* (38), 27862-27872.

56. McCrate, N. E.; Varner, M. E.; Kim, K. I.; Nagan, M. C., Molecular dynamics simulations of human tRNA (Lys,3)(UUU) : the role of modified bases in mRNA recognition. *Nucleic Acids Research* **2006,** *34* (19), 5361-5368.

57. Kirschner, K. N.; Lewin, A. H.; Bowen, J. P., Molecular mechanics force-field development for amino acid zwitterions. *Journal of Computational Chemistry* **2003,** *24* (1), 111-128.

58. Hillson, S. D.; Smith, E.; Zeldin, M.; Parish, C. A., Cages, baskets, ladders, and tubes: Conformational studies of polyhedral oligomeric silsesquioxanes. *J. Phys. Chem. A* **2005,** *109* (37), 8371-8378.

59. Brzostowska, E. M.; Hoffmann, R.; Parish, C. A., Tuning the bergman cyclization by introduction of metal fragments at various positions of the enediyne. Metalla-Bergman cyclizations. *Journal of the American Chemical Society* **2007,** *129* (14), 4401-4409.

60. Day, M. B.; Kirschner, K. N.; Shields, G. C., Global search for minimum energy (H2O)(n) clusters, n=3-5. *J. Phys. Chem. A* **2005,** *109* (30), 6773-6778.

61. Gomez, J. A.; Tucker, A. K.; Shepherd, T. D.; Thompson, W. H., Conformational free energies of 1,2-dichloroethane in nanoconfined methanol. *J. Phys. Chem. B* **2005,** *109* (37), 17479-17487.

62. Liptak, M. D.; Shields, G. C., Comparison of density functional theory predictions of gas-phase deprotonation data. *International Journal of Quantum Chemistry* **2005,** *105* (6), 580-587.

63. Pickard, F. C.; Dunn, M. E.; Shields, G. C., Comparison of model chemistry and density functional theory thermochemical predictions with experiment for formation of ionic clusters of the ammonium cation complexed with water and ammonia; Atmospheric implications. *J. Phys. Chem. A* **2005,** *109* (22), 4905-4910.

64. Zhan, C. G.; Deng, S. X.; Skiba, J. G.; Hayes, B. A.; Tschampel, S. M.; Shields, G. C.; Landry, D. W., First-principle studies of intermolecular and intramolecular catalysis of protonated cocaine. *Journal of Computational Chemistry* **2005,** *26* (10), 980-986.

65. Allodi, M. A.; Dunn, M. E.; Livada, J.; Kirschner, K. N.; Shields, G. C., Do hydroxyl radical-water clusters, OH(H2O)(n), n=1-5, exist in the atmosphere? *J. Phys. Chem. A* **2006,** *110* (49), 13283-13289.

66. Alongi, K. S.; Dibble, T. S.; Shields, G. C.; Kirschner, K. N., Exploration of the potential energy surfaces, prediction of atmospheric concentrations, and prediction of vibrational spectra for the HO2 (H2O)n (n=1-2) hydrogen bonded complexes. *J. Phys. Chem. A* **2006,** *110* (10), 3686-3691.

67. Dunn, M. E.; Evans, T. M.; Kirschner, K. N.; Shields, G. C., Prediction of accurate anharmonic experimental vibrational frequencies for water clusters, (H2O)(n), n=2-5. *J. Phys. Chem. A* **2006,** *110* (1), 303-309.

68. Pickard, F. C.; Griffith, D. R.; Ferrara, S. J.; Liptak, M. D.; Kirschner, K. N.; Shields, G. C., CCSD(T), W1, and other model chemistry predictions for gas-phase deprotonation reactions. *International Journal of Quantum Chemistry* **2006,** *106* (15), 3122-3128.

69. Pickard, F. C.; Shepherd, R. L.; Gillis, A. E.; Dunn, M. E.; Feldgus, S.; Kirschner, K. N.; Shields, G. C.; Manoharan, M.; Alabugin, I. V., Ortho effect in the Bergman cyclization: Electronic and steric effects in hydrogen abstraction by 1-substituted naphthalene 5,8-diradicals. *J. Phys. Chem. A* **2006,** *110* (7), 2517-2526.

70. Kirschner, K. N.; Hartt, G. M.; Evans, T. M.; Shields, G. C., In search of CS2(H2O)(n=1-4) clusters. *J. Chem. Phys.* **2007,** *126* (15).

71. Kirschner, K. N.; Lexa, K. W.; Salisburg, A. M.; Alser, K. A.; Joseph, L.; Andersen, T. T.; Bennett, J. A.; Jacobson, H. I.; Shields, G. C., Computational design and experimental discovery of an antiestrogenic peptide derived from alpha-fetoprotein. *Journal of the American Chemical Society* **2007,** *129* (19), 6263-6268.

72. Lexa, K. W.; Alser, K. A.; Salisburg, A. M.; Ellens, D. J.; Hernandez, L.; Bono, S. J.; Michael, H. C.; Derby, J. R.; Skiba, J. G.; Feldgus, S.; Kirschner, K. N.; Shields, G. C., The search for low energy conformational families of small peptides: Searching for active conformations of small peptides in the absence of a known receptor. *International Journal of Quantum Chemistry* **2007,** *107* (15), 3001-3012.

73. Baffour-Awuah, N. Y.; Fedeles, F.; Zimmer, M., Structural features responsible for GFPuv and S147P-GFP's improved fluorescence. *Chemical Physics* **2005,** *310* (1-3), 25-31.

74. Baffour-Awuah, N. Y.; Maddalo, S.; Zimmer, M., Photophysics and chromophore cavity analysis of green fluorescent protein. *Febs Journal* **2005,** *272*, 22-22.

75. Branchini, B. R.; Southworth, T. L.; Murtiashaw, M. H.; Wilkinson, S. R.; Khattak, N. F.; Rosenberg, J. C.; Zimmer, M., Mutagenesis evidence that the partial reactions of firefly bioluminescence are catalyzed by different conformations of the luciferase C-terminal domain. *Biochemistry* **2005,** *44* (5), 1385-1393.

76. Maddalo, S. L.; Zimmer, M., The role of the protein matrix in green fluorescent protein fluorescence. *Photochemistry and Photobiology* **2006,** *82* (2), 367-372.

77. Mbofana, C.; Zimmer, M., Effect of the methyl-coenzyme-m reductase protein matrix on the hole-size and nonplanar deformations of coenzyme F430. *Inorganic Chemistry* **2006,** *45* (6), 2598-2602.

78. Branchini, B. R.; Ablamsky, D. M.; Rosenman, J. M.; Uzasci, L.; Southworth, T. L.; Zimmer, M., Synergistic mutations produce blue-shifted bioluminescence in firefly luciferase. *Biochemistry* **2007,** *46* (48), 13847-13855.

79. Seckute, J.; Menke, J. L.; Emnett, R. J.; Patterson, E. V.; Cramer, C. J., Ab initio molecular orbital and density functional studies on the solvolysis of sarin and O,S-dimethyl methylphosphonothiolate, a VX-like compound. *J. Org. Chem.* **2005,** *70* (22), 8649-8660.

80. Jay, A. N.; Daniel, K. A.; Patterson, E. V., Atom-centered density matrix propagation calculations on the methyl transfer from CH3Cl to NH3: Gas-phase and continuum-solvated trajectories. *J. Chem. Theory Comput.* **2007,** *3* (2), 336-343.

81. Menke, J. L.; Patterson, E. V., Quantum mechanical calculations on the reaction of ethoxide anion with O,S-dimethyl methylphosphonothiolate. *Theochem-J. Mol. Struct.* **2007,** *811* (1-3), 281-291.

82. Szczepanska, A.; Espartero, J. L.; Moreno-Vargas, A. J.; Carmona, A. T.; Robina, I.; Remmert, S.; Parish, C., Synthesis and Conformational Analysis of Novel Trimeric Maleimide Cross-Linking Reagents. *J. Org. Chem.* **2007,** *72*, 6776-6785.

83. Lauer, M. G.; Leslie, J. W.; Mynar, A.; Stamper, S. A.; Martinez, A. D.; Bray, A. J.; Negassi, S.; McDonald, K.; Ferraris, E.; Muzny, A.; McAvoy, S.; Miller, C. P.; Walters, K. A.; Russell, K. C.; Wang, E.; Nuez, B.; Parish, C., Synthesis, Spectroscopy, and Theoretical Calculations for a Series of Push-Pull [14]-Pyridoannulenes. *The Journal of Organic Chemistry* **2008,** *73* (2), 474-484.

84. Donald, K. J.; Hoffmann, R., Solid memory: Structural preferences in group 2 dihalide monomers, dimers, and solids. *Journal of the American Chemical Society* **2006,** *128* (34), 11236-11249.

85. Merino, G.; Donald, K. J.; D'Acchioli, J. S.; Hoffmann, R., The many ways to have a quintuple bond. *Journal of the American Chemical Society* **2007,** *129* (49), 15295-15302.

86. Wang, E. B.; Parish, C. A.; Lischka, H., An extended multireference study of the electronic states of para-benzyne. *The Journal of Chemical Physics* **2008,** *129* (4), 044306-8.

87. Cafiero, M.; Adamowicz, L., Non–Born–Oppenheimer calculations of the ground state of H3. *International Journal of Quantum Chemistry* **2007,** *107* (14), 2679-2686.

88. Hofto, L.; Hofto, M.; Cross, J.; Cafiero, M., Using simple molecular orbital calculations to predict disease: fast DFT methods applied to enzymes implicated in PKU, Parkinson's disease and Obsessive Compulsive Disorder. *AIP Conference Proceedings* **2007,** *940* (1), 127-136.

89. Hofto, M. E.; Cross, J. N.; Cafiero, M., Interaction Energies between Tetrahydrobiopterin Analogues and Aromatic Residues in Tyrosine Hydroxylase and Phenylalanine Hydroxylase. *The Journal of Physical Chemistry B* **2007,** *111* (32), 9651-9654.

90. Hofto, M. E.; Godfrey-Kittle, A.; Cafiero, M., Substrate-protein interaction energy in the enzyme phenylalanine hydroxylase: DFT and ab initio results. *Journal of Molecular Structure: THEOCHEM* **2007,** *809* (1‚Äì3), 125-130.

91. Van Sickle, K.; Culberson, L. M.; Holzmacher, J. L.; Cafiero, M., Evaluation of density functional theory methods for the electronic interactions between indole and substituted benzene: Applications to horseradish peroxidase. *International Journal of Quantum Chemistry* **2007,** *107* (6), 1523-1531.

92. Pavanello, M.; Cafiero, M.; Bubin, S.; Adamowicz, L., Accurate Born-Oppenheimer calculations of the low-lying c(3)Sigma(+)(g) and a(3)Sigma(+)(u) excited states of helium dimer. *International Journal of Quantum Chemistry* **2008,** *108* (12), 2291-2298.

93. Cerpa, E.; Tenorio, F. J.; Contreras, M.; Villanueva, M.; Beltran, H. I.; Heine, T.; Donald, K. J.; Merino, G., Pentadienyl Complexes of Alkali Metals: Structure and Bonding. *Organometallics* **2008,** *27* (5), 827-833.

94. Jambor, R.; Kašná, B.; Kirschner, K. N.; Schürmann, M.; Jurkschat, K., [{2,6-(Me2NCH2)2C6H3}Sn]2: An Intramolecularly Coordinated Diorganodistannyne. *Angewandte Chemie International Edition* **2008,** *47* (9), 1650-1653.

95. Kirschner, K. N.; Yongye, A. B.; Tschampel, S. M.; González-Outeiriño, J.; Daniels, C. R.; Foley, B. L.; Woods, R. J., GLYCAM06: A generalizable biomolecular force field. Carbohydrates. *Journal of Computational Chemistry* **2008,** *29* (4), 622-655.

96. Zhong, H.; Kirschner, K. N.; Lee, M.; Bowen, J. P., Binding free energy calculation for duocarmycin/DNA complex based on the QPLD-derived partial charge model. *Bioorganic & Medicinal Chemistry Letters* **2008,** *18* (2), 542-545.

97. Lemay, N. P.; Morgan, A. L.; Archer, E. J.; Dickson, L. A.; Megley, C. M.; Zimmer, M., The role of the tight-turn, broken hydrogen bonding, Glu222 and Arg96 in the post-translational green fluorescent protein chromophore formation. *Chemical Physics* **2008,** *348* (1‚Äì3), 152-160.

98. Megley, C. M.; Dickson, L. A.; Maddalo, S. L.; Chandler, G. J.; Zimmer, M., Photophysics and Dihedral Freedom of the Chromophore in Yellow, Blue, and Green Fluorescent Protein. *The Journal of Physical Chemistry B* **2008,** *113* (1), 302-308.

99. Dunn, M. E.; Shields, G. C.; Takahashi, K.; Skodje, R. T.; Vaida, V., Experimental and Theoretical Study of the OH Vibrational Spectra and Overtone Chemistry of Gas-Phase Vinylacetic Acid. *The Journal of Physical Chemistry A* **2008,** *112* (41), 10226-10235.

100. Hartt, G. M.; Shields, G. C.; Kirschner, K. N., Hydration of OCS with One to Four Water Molecules in Atmospheric and Laboratory Conditions. *The Journal of Physical Chemistry A* **2008,** *112* (19), 4490-4495.

101. Sherer, E. C.; Kirschner, K. N.; Pickard, F. C.; Rein, C.; Feldgus, S.; Shields, G. C., Efficient and Accurate Characterization of the Bergman Cyclization for Several Enediynes Including an Expanded Substructure of Esperamicin A1. *The Journal of Physical Chemistry B* **2008,** *112* (51), 16917-16934.

102. Shields, G. C.; Kirschner, K. N., The Limitations of Certain Density Functionals in Modeling Neutral Water Clusters. *Synthesis and Reactivity in Inorganic, Metal-Organic, and Nano-Metal Chemistry* **2008,** *38* (1), 32-39.

103. Zimmer, M., Are classical molecular mechanics calculations still useful in bioinorganic simulations? *Coordination Chemistry Reviews* **2009,** *253* (5-6), 817-826.

104. Zimmer, M., GFP: from jellyfish to the Nobel prize and beyond. *Chem. Soc. Rev.* **2009,** *38* (10), 2823-2832.

105. Remmert, S.; Hollis, H.; Parish, C. A., Conformational analysis of trimeric maleimide substituted 1,5,9-triazacyclododecane HIV fusion scaffolds. *Bioorganic & Medicinal Chemistry* **2009,** *17* (3), 1251-1258.

106. Remmert, S.; Parish, C., Energetic analyses of chair and boat conformations of maleimide substituted cyclohexane derivatives. *Journal of Computational Chemistry* **2009,** *30* (6), 992-998.

107. Joseph, L. C.; Bennett, J. A.; Kirschner, K. N.; Shields, G. C.; Hughes, J.; Lostritto, N.; Jacobson, H. I.; Andersen, T. T., Antiestrogenic and anticancer activities of peptides derived from the active site of alpha-fetoprotein. *Journal of Peptide Science* **2009,** *15* (4), 319-325.

108. Salisburg, A. M.; Deline, A. L.; Lexa, K. W.; Shields, G. C.; Kirschner, K. N., Ramachandran-type plots for glycosidic linkages: Examples from molecular dynamic simulations using the Glycam06 force field. *Journal of Computational Chemistry* **2009,** *30* (6), 910-921.

109. Shields, G. C., Computational approaches for the design of peptides with anti-breast cancer properties. *Future Medicinal Chemistry* **2009,** *1* (1), 201-212.

110. Daniel, K. A.; Kopff, L. A.; Patterson, E. V., Computational studies on the solvolysis of the chemical warfare agent VX. *Journal of Physical Organic Chemistry* **2008,** *21* (4), 321-328.

111. Maki, B. E.; Patterson, E. V.; Cramer, C. J.; Scheidt, K. A., Impact of Solvent Polarity on N-Heterocyclic Carbene-Catalyzed beta-Protonations of Homoenolate Equivalents. *Org. Lett.* **2009,** *11* (17), 3942-3945.

112. Seburg, R. A.; Patterson, E. V.; McMahon, R. J., Structure of Triplet Propynylidene (HCCCH) as Probed by IR, UV/vis, and EPR Spectroscopy of Isotopomers. *Journal of the American Chemical Society* **2009,** *131* (26), 9442-9455.

113. Hofto, L. R.; Lee, C. E.; Cafiero, M., The Importance of Aromatic-Type Interactions in Serotonin Synthesis: Protein-Ligand Interactions in Tryptophan Hydroxylase and Aromatic Amino Acid Decarboxylase. *Journal of Computational Chemistry* **2009,** *30* (7), 1111-1115.

114. Kee, E. A.; Livengood, M. C.; Carter, E. E.; McKenna, M.; Cafiero, M., Aromatic Interactions in the Binding of Ligands to HMGCoA Reductase. *J. Phys. Chem. B* **2009,** *113* (44), 14810-14815.

115. Irving, D. L.; Padgett, C. W.; Brenner, D. W., Coupled molecular dynamics/continuum simulations of Joule heating and melting of isolated copper-aluminum asperity contacts. *Modelling and Simulation in Materials Science and Engineering* **2009,** *17* (1), 015004.

116. Padgett, C.; Saad, A., Genetic Algorithms in Chemistry: Success or Failure Is in the Genes. In *Applications of Soft Computing: From Theory to Praxix*, Mehnen, J.; Köppen, M.; Saad, A.; Tiwari, A., Eds. Springer Berlin / Heidelberg: 2009; Vol. 58, pp 181-189.

117. Padgett, C. W.; Gutt, K. J.; Whiteside, T. S., Computational studies on the mechanical properties of diamond nanotoroids. *Computational Materials Science* **2009,** *46* (2), 491-494.

118. Cerpa, E.; Krapp, A.; Flores-Moreno, R.; Donald, K. J.; Merino, G., Influence of Endohedral Confinement on the Electronic Interaction between He atoms: A He2@C20H20 Case Study. *Chemistry – A European Journal* **2009,** *15* (8), 1985-1990.

119. Craciun, S.; Donald, K. J., Radical Bonding: Structure and Stability of Bis(Phenalenyl) Complexes of Divalent Metals from across the Periodic Table. *Inorganic Chemistry* **2009,** *48* (13), 5810-5819.

120. Donald, K. J.; Hargittai, M.; Hoffmann, R., Group 12 Dihalides: Structural Predilections from Gases to Solids. *Chemistry – A European Journal* **2009,** *15* (1), 158-177.

121. Michael, L. A.; Chenault, J. A.; Miller, B. R.; Knolhoff, A. M.; Nagan, M. C., Water, Shape Recognition, Salt Bridges, and Cation-Pi Interactions Differentiate Peptide Recognition of the HIV Rev-Responsive Element. *Journal of Molecular Biology* **2009,** *392* (3), 774-786.

122. Gao, D., Acidities of Water and Methanol in Aqueous Solution and DMSO. *Journal of Chemical Education* **2009,** *86* (7), 864.

123. Samma, A. A.; Johnson, C. K.; Song, S. A.; Alvarez, S.; Zimmer, M., On the Origin of Fluorescence in Bacteriophytochrome Infrared Fluorescent Proteins. *J. Phys. Chem. B* **2010,** *114* (46), 15362-15369.

124. Donald, K. J.; Wittmaack, B. K.; Crigger, C., Tuning sigma-Holes: Charge Redistribution in the Heavy (Group 14) Analogues of Simple and Mixed Halomethanes Can Impose Strong Propensities for Halogen Bonding. *J. Phys. Chem. A* **2010,** *114* (26), 7213-7222.

125. Ghosh, K.; Saha, I.; Masanta, G.; Wang, E. B.; Parish, C. A., Triphenylamine-based receptor for selective recognition of dicarboxylates. *Tetrahedron Lett.* **2010,** *51* (2), 343-347.

126. Hamm, M. L.; Parker, A. J.; Steele, T. W. E.; Carman, J. L.; Parish, C. A., Oligonucleotide Incorporation and Base Pair Stability of 9-Deaza-2'-deoxyguanosine, an Analogue of 8-Oxo-2 '-deoxyguanosine. *J. Org. Chem.* **2010,** *75* (16), 5661-5669.

127. Wang, E. B.; Parish, C. A., Conformational Analysis of a Model for the trans-Fused FGH Ether Rings in Brevetoxin A. *J. Org. Chem.* **2010,** *75* (5), 1582-1588.

128. Martinez-Guajardo, G.; Donald, K. J.; Wittmaack, B. K.; Vazquez, M. A.; Merino, G., Shorter Still: Compressing C-C Single Bonds. *Org. Lett.* **2010,** *12* (18), 4058-4061.

129. Alongi, K. S.; Shields, G. C., Theoretical Calculations of Acid Dissociation Constants: A Review Article. In *Annual Reports in Computational Chemistry, Vol 6*, Wheeler, R. A., Ed. Elsevier Science Bv: Amsterdam, 2010; Vol. 6, pp 113-138.

130. Morrell, T. E.; Shields, G. C., Atmospheric Implications for Formation of Clusters of Ammonium and 1-10 Water Molecules. *J. Phys. Chem. A* **2010,** *114* (12), 4266-4271.

131. Shields, R. M.; Temelso, B.; Archer, K. A.; Morrell, T. E.; Shields, G. C., Accurate Predictions of Water Cluster Formation, (H(2)O)(n=2-10). *J. Phys. Chem. A* **2010,** *114* (43), 11725-11737.

132. Gomez, M. A.; Chunduru, M.; Chigweshe, L.; Fletcher, K. M., The effect of dopant at the Zr site on the proton conduction pathways of SrZrO(3): An orthorhombic perovskite. *J. Chem. Phys.* **2010,** *133* (6), 7.

133. Gomez, M. A.; Chunduru, M.; Chigweshe, L.; Foster, L.; Fensin, S. J.; Fletcher, K. M.; Fernandez, L. E., The effect of yttrium dopant on the proton conduction pathways of BaZrO(3), a cubic perovskite. *J. Chem. Phys.* **2010,** *132* (21), 8.

134. Utkov, H.; Livengood, M.; Cafiero, M., Using Density Functional Theory methods for modeling induction and dispersion interactions in ligand-protein complexes. In *Annual Reports in Computational Chemistry* Elsevier: 2010; Vol. 6, p 97.

135. Van Sickle, K.; Shroyer, M. C.; Cafiero, M., Relative stability of complexes of six-carbon-rings with variable numbers of double bonds: DFT and ab initio results. *Theochem-J. Mol. Struct.* **2010,** *941* (1-3), 78-84.

136. Sung, J. C.; Van Wynsberghe, A. W.; Amaro, R. E.; Li, W. W.; McCammon, J. A., Role of Secondary Sialic Acid Binding Sites in Influenza N1 Neuraminidase. *Journal of the American Chemical Society* **2010,** *132* (9), 2883-2885.

137. Van Wynsberghe, A. W.; Cui, Q., Conservation and Variation of Structural Flexibility in Protein Families. *Structure* **2010,** *18* (3), 281-283.

138. Crill, J. W.; Ji, X.; Irving, D. L.; Brenner, D. W.; Padgett, C. W., Atomic and multi-scale modeling of non-equilibrium dynamics at metal-metal contacts. *Modelling and Simulation in Materials Science and Engineering* **2010,** *18* (3), 034001.

139. Nivens, D. A.; Padgett, C. W.; Chase, J. M.; Verges, K. J.; Jamieson, D. S., Art, Meet Chemistry; Chemistry, Meet Art: Case Studies, Current Literature, and Instrumental Methods Combined To Create a Hands-On Experience for Nonmajors and Instrumental Analysis Students. *Journal of Chemical Education* **2010,** *87* (10), 1089-1093.

140. Whiteside, T. S.; Priest, M. A.; Padgett, C. W., Enthalpies of formation of methyl substituted naphthalenes. *Thermochim. Acta* **2010,** *510* (1-2), 17-23.

141. Menke, J. L.; Patterson, E. V.; McMahon, R. J., Effects of Cyano Substituents on Cyclobutadiene and Its Isomers. *J. Phys. Chem. A* **2010,** *114* (22), 6431-6437.

142. Tvedte, L. M.; Smith, K. L.; Patterson, E. V.; Baughman, R. G., 2-Amino-5-(3,4-dimethoxybenzylidene)-1-methylimidazol-4(5H)-one N,N-dimethylformamide monosolvate. *Acta Crystallogr. Sect. C-Cryst. Struct. Commun.* **2010,** *66*, O101-O103.

143. Temelso, B.; Archer, K. A.; Shields, G. C., Benchmark Structures and Binding Energies of Small Water Clusters with Anharmonicity Corrections. *J. Phys. Chem. A* **2011,** *115* (43), 12034-12046.

144. Temelso, B.; Shields, G. C., The Role of Anharmonicity in Hydrogen-Bonded Systems: The Case of Water Clusters. *J. Chem. Theory Comput.* **2011,** *7* (9), 2804-2817.

145. Ong, W. J. H.; Alvarez, S.; Leroux, I. E.; Shahid, R. S.; Samma, A. A.; Peshkepija, P.; Morgan, A. L.; Mulcahy, S.; Zimmer, M., Function and structure of GFP-like proteins in the protein data bank. *Molecular Biosystems* **2011,** *7* (4), 984-992.

146. Utkov, H. E.; Price, A. M.; Cafiero, M., MP2, density functional theory, and semi-empirical calculations of the interaction energies between a series of statin-drug-like molecules and the HMG-CoA reductase active site. *Comput. Theor. Chem.* **2011,** *967* (1), 171-178.

147. Sinko, W.; de Oliveira, C.; Williams, S.; Van Wynsberghe, A.; Durrant, J. D.; Cao, R.; Oldfield, E.; McCammon, J. A., Applying Molecular Dynamics Simulations to Identify Rarely Sampled Ligand-bound Conformational States of Undecaprenyl Pyrophosphate Synthase, an Antibacterial Target. *Chem. Biol. Drug Des.* **2011,** *77* (6), 412-420.

148. Tsutakawa, S. E.; Van Wynsberghe, A. W.; Freudenthal, B. D.; Weinacht, C. P.; Gakhar, L.; Washington, M. T.; Zhuang, Z. H.; Tainer, J. A.; Ivanov, I., Solution X-ray scattering combined with computational modeling reveals multiple conformations of covalently bound ubiquitin on PCNA. *Proc. Natl. Acad. Sci. U. S. A.* **2011,** *108* (43), 17672-17677.

149. Durham, C. R.; Chase, J. M.; Nivens, D. A.; Baird, W. H.; Padgett, C. W., Chemical Environment Effects on K beta/K alpha Intensity Ratio: An X-ray Fluorescence Experiment on Periodic Trends. *Journal of Chemical Education* **2011,** *88* (6), 819-821.

150. Priest, M. A.; Padgett, L. W.; Padgett, C. W., Demonstrating the Temperature Dependence of Density via Construction of a Galilean Thermometer. *Journal of Chemical Education* **2011,** *88* (7), 983-985.

151. Donald, K. J.; Bober, M., Predicting the Relative Stability of Simple versus ansa-Sandwich Systems Across Groups: Structure, Bonding, and (In)Stability in Tris(sandwich)benzene Complexes. *Chem.-Eur. J.* **2011,** *17* (6), 1936-1945.

152. Martinez-Guajardo, G.; Donald, K. J.; Wittmaack, B. K.; Vazquez, M. A.; Merino, G., Shorter Still: Compressing C-C Single Bonds. (vol 12, pg 4058, 2010). *Org. Lett.* **2011,** *13* (1), 172-172.

153. Perez-Peralta, N.; Contreras, M.; Tiznado, W.; Stewart, J.; Donald, K. J.; Merino, G., Stabilizing carbon-lithium stars. *Phys. Chem. Chem. Phys.* **2011,** *13* (28), 12975-12980.

154. Wittmaack, B. K.; Crigger, C.; Guarino, M.; Donald, K. J., Charge Saturation and Neutral Substitutions in Halomethanes and Their Group 14 Analogues. *J. Phys. Chem. A* **2011,** *115* (31), 8743-8753.

155. Mueller, R. M.; North, M. A.; Yang, C.; Hati, S.; Bhattacharyya, S., Interplay of Flavin's Redox States and Protein Dynamics: An Insight from QM/MM Simulations of Dihydronicotinamide Riboside Quinone Oxidoreductase 2. *The Journal of Physical Chemistry B* **2011,** *115* (13), 3632-3641.

156. Song, X.; Parish, C. A., A Mechanistic Study of the 2-Thienylmethyl + HO2 Radical Recombination Reaction. *J. Phys. Chem. A* **2011,** *115* (50), 14546-14557.

157. Ghosh, K.; Sen, T.; Patra, A.; Mancini, J. S.; Cook, J. M.; Parish, C. A., (rac)-1,1'-Binaphthyl-Based Simple Receptors Designed for Fluorometric Discrimination of Maleic and Fumaric Acids. *J. Phys. Chem. B* **2011,** *115* (26), 8597-8608.

158. Song, X. L.; Parish, C. A., Pyrolysis Mechanisms of Thiophene and Methylthiophene in Asphaltenes. *J. Phys. Chem. A* **2011,** *115* (13), 2882-2891.

159. Husar, D. E.; Temelso, B.; Ashworth, A. L.; Shields, G. C., Hydration of the Bisulfate Ion: Atmospheric Implications. *J. Phys. Chem. A* **2012,** *116* (21), 5151-5163.

160. Pérez, C.; Muckle, M. T.; Zaleski, D. P.; Seifert, N. A.; Temelso, B.; Shields, G. C.; Kisiel, Z.; Pate, B. H., Structures of Cage, Prism, and Book Isomers of Water Hexamer from Broadband Rotational Spectroscopy. *Science* **2012,** *336*, 897-901.

161. Temelso, B.; Morrell, T. E.; Shields, R. M.; Allodi, M. A.; Wood, E. K.; Kirschner, K. N.; Castonguay, T. C.; Archer, K. A.; Shields, G. C., Quantum Mechanical Study of Sulfuric Acid Hydration: Atmospheric Implications. *J. Phys. Chem. A* **2012,** *116* (9), 2209-2224.

162. Temelso, B.; Phan, T. N.; Shields, G. C., Computational Study of the Hydration of Sulfuric Acid Dimers: Implications for Acid Dissociation and Aerosol Formation. *J. Phys. Chem. A* **2012,** *116* (39), 9745-9758.

163. Klimavicz, J. S.; Mike, J. F.; Bhuwalka, A.; Tomlinson, A. L.; Jeffries-El, M., Synthesis of benzobisoxazole-based D-pi-A-pi-D organic chromophores with variable optical and electronic properties. *Pure and Applied Chemistry* **2012,** *84* (4), 991-1004.

164. Kobilka, B. M.; Dubrovskiy, A. V.; Ewan, M. D.; Tomlinson, A. L.; Larock, R. C.; Chaudhary, S.; Jeffries-El, M., Synthesis of 3,7-diiodo-2,6-di(thiophen-2-yl)benzo 1,2-b:4,5-b ' difurans: functional building blocks for the design of new conjugated polymers. *Chemical Communications* **2012,** *48* (71), 8919-8921.

165. Baltrusaitis, J.; Patterson, E. V.; Hatch, C., Computational Studies of CO2 Activation via Photochemical Reactions with Reduced Sulfur Compounds. *J. Phys. Chem. A* **2012,** *116* (37), 9331-9339.

166. Shepherd, T. D.; Koc, M. A.; Molinero, V., The Quasi-Liquid Layer of Ice under Conditions of Methane Clathrate Formation. *Journal of Physical Chemistry C* **2012,** *116* (22), 12172-12180.

167. Gomez, M. A.; Shepardson, D.; Nguyen, L. T.; Kehinde, T., Periodic long range proton conduction pathways in pseudo-cubic and orthorhombic perovskites. *Solid State Ionics* **2012,** *213*, 8-13.

168. Fisher, S. Q.; Weck, M.; Landers, J. E.; Emrich, J.; Middleton, S. A.; Cox, J.; Gentile, L.; Parish, C. A., Evidence that the kinesin light chain domain contains tetratricopeptide repeat units. *Journal of Structural Biology* **2012,** *177* (3), 602-612.

169. Parker, A. J.; Stewart, J.; Donald, K. J.; Parish, C. A., Halogen Bonding in DNA Base Pairs. *Journal of the American Chemical Society* **2012,** *134* (11), 5165-5172.

170. Song, X.; Fanelli, M. G.; Cook, J. M.; Bai, F.; Parish, C. A., Mechanisms for the Reaction of Thiophene and Methylthiophene with Singlet and Triplet Molecular Oxygen. *J. Phys. Chem. A* **2012,** *116* (20), 4934-4946.

171. Castro, A. C.; Martinez-Guajardo, G.; Johnson, T.; Ugalde, J. M.; Wu, Y.-b.; Mercero, J. M.; Heine, T.; Donald, K. J.; Merino, G., CBe5E- (E = Al, Ga, In, Tl): planar pentacoordinate carbon in heptaatomic clusters. *Phys. Chem. Chem. Phys.* **2012,** *14* (43), 14764-14768.

172. Crigger, C.; Wittmaack, B. K.; Tawfik, M.; Merino, G.; Donald, K. J., Plane and simple: planar tetracoordinate carbon centers in small molecules. *Phys. Chem. Chem. Phys.* **2012,** *14* (43), 14775-14783.

173. Osorio, E.; Villalobos, V.; Santos, J. C.; Donald, K. J.; Merino, G.; Tiznado, W., Structure and stability of the Si4Lin (n=1-7) binary clusters. *Chemical Physics Letters* **2012,** *522*, 67-71.

174. Sanford, B.; Cao, B.; Johnson, J. M.; Zimmerman, K.; Strom, A. M.; Mueller, R. M.; Bhattacharyya, S.; Musier-Forsyth, K.; Hati, S., Role of Coupled Dynamics in the Catalytic Activity of Prokaryotic-like Prolyl-tRNA Synthetases. *Biochemistry* **2012,** *51* (10), 2146-2156.

175. Li, B.; Shahid, R.; Peshkepija, P.; Zimmer, M., Water diffusion in and out of the beta-barrel of GFP and the fast maturing fluorescent protein, TurboGFP. *Chemical Physics* **2012,** *392* (1), 143-148.

176. Zimmer, M., What does it take to improve existing fluorescent proteins for in vivo imaging applications? *Methods in molecular biology (Clifton, N.J.)* **2012,** *872*, 235-41.

177. Knauf, R. R.; Helminiak, H. M.; Wrass, J. P.; Gallert, T. M.; Phillips, J. A., Structural and energetic properties of alkylfluoride-BF3 complexes in the gas phase and condensed-phase media: computations and matrix infrared spectroscopy. *Journal of Physical Organic Chemistry* **2012,** *25* (6), 493-501.

178. Pérez, C.; Lobsiger, S.; Seifert, N. A.; Zaleski, D. P.; Temelso, B.; Shields, G. C.; Kisiel, Z.; Pate, B. H., Broadband Fourier transform rotational spectroscopy for structure determination: The water heptamer. *Chemical Physics Letters* **2013,** *571*, 1- 15.

179. Shields, G. C.; Seybold, P. G., *Computational Approaches for the Prediction of pKa Values*. CRC Press: 2013.

180. Temelso, B.; Koddermann, T.; Kirschner, K. N.; Klein, K.; Shields, G. C., Structure and thermodynamics of H3O+(H2O)8 clusters: A combined molecular dynamics and quantum mechanics approach. *Comput. Theor. Chem.* **2013,** *1021*, 240-248.

181. Buchberger, A. R.; Danforth, S. J.; Bloomgren, K. M.; Rohde, J. A.; Smith, E. L.; Gardener, C. C. A.; Phillips, J. A., Condensed-Phase Effects on the Structural Properties of FCH2CN-BF3 and ClCH2CN-BF3: A Matrix-Isolation and Computational Study. *J. Phys. Chem. B* **2013,** *117* (39), 11687-11696.

182. Murdachaew, G.; Varner, M. E.; Phillips, L. F.; Finlayson-Pitts, B. J.; Gerber, R. B., Nitrogen dioxide at the air-water interface: trapping, absorption, and solvation in the bulk and at the surface. *Phys. Chem. Chem. Phys.* **2013,** *15* (1), 204-212.

183. Hu, H. H.; Shepherd, T. D., Using POGIL to Help Students Learn to Program. *Acm Transactions on Computing Education* **2013,** *13* (3).

184. Qu, S.; Kolodziej, E. P.; Long, S. A.; Gloer, J. B.; Patterson, E. V.; Baltrusaitis, J.; Jones, G. D.; Benchetler, P. V.; Cole, E. A.; Kimbrough, K. C.; Tarnoff, M. D.; Cwiertny, D. M., Product-to-Parent Reversion of Trenbolone: Unrecognized Risks for Endocrine Disruption. *Science* **2013,** *342* (6156), 347-351.

185. Witts, R. N.; Hopson, E. C.; Koballa, D. E.; Van Boening, T. A.; Hopkins, N. H.; Patterson, E. V.; Nagan, M. C., Backbone-Base Interactions Critical to Quantum Stabilization of Transfer RNA Anticodon Structure. *J. Phys. Chem. B* **2013,** *117* (25), 7489-7497.

186. Kinnel, R., B. ; Van Wynsberghe, A., W. ; Rosenstein, I., J. ; Brewer, K., S. ; Cotten, M.; Shields, G., C. ; Borton, C., J. ; Senior, S., Z. ; Rahn, G., S. ; Elgren, T., E. , A Departmental Focus on High Impact Undergraduate Research Experiences. In *Developing and Maintaining a Successful Undergraduate Research Program*, American Chemical Society: 2013; Vol. 1156, pp 5-22.

187. Gomez, M. A.; Liu, F.-J., Protons in Al doped BaZrO3 escape dopant traps to access long range proton conduction highways. *Solid State Ionics* **2013,** *252*, 40-47.

188. Contreras, M.; Osorio, E.; Ferraro, F.; Puga, G.; Donald, K. J.; Harrison, J. G.; Merino, G.; Tiznado, W., Isomerization Energy Decomposition Analysis for Highly Ionic Systems: Case Study of Starlike E5Li7+ Clusters. *Chem.-Eur. J.* **2013,** *19* (7), 2305-2310.

189. Donald, K. J.; Kovac, J., The Scientist's Education and a Civic Conscience. *Science and Engineering Ethics* **2013,** *19* (3), 1229-1240.

190. Donald, K. J.; Tawfik, M., The Weak Helps the Strong: Sigma-Holes and the Stability of MF4 center dot Base Complexes. *J. Phys. Chem. A* **2013,** *117* (51), 14176-14183.

191. Osorio, E.; Vasquez, A.; Florez, E.; Mondragon, F.; Donald, K. J.; Tiznado, W., Theoretical design of stable small aluminium-magnesium binary clusters. *Phys. Chem. Chem. Phys.* **2013,** *15* (6), 2222-2229.

192. Tlach, B. C.; Tomlinson, A. L.; Ryno, A. G.; Knoble, D. D.; Drochner, D. L.; Krager, K. J.; Jeffries-El, M., Influence of Conjugation Axis on the Optical and Electronic Properties of Aryl-Substituted Benzobisoxazoles. *J. Org. Chem.* **2013,** *78* (13), 6570-6581.

193. Eggimann, B. L.; Vostrikov, V. V.; Veglia, G.; Siepmann, J. I., Modeling helical proteins using residual dipolar couplings, sparse long-range distance constraints and a simple residue-based force field. *Theoretical Chemistry Accounts* **2013,** *132* (10).

194. Lindsey, R. K.; Rafferty, J. L.; Eggimann, B. L.; Siepmann, J. I.; Schure, M. R., Molecular simulation studies of reversed-phase liquid chromatography. *Journal of Chromatography A* **2013,** *1287*, 60-82.

195. Johnson, J. M.; Sanford, B. L.; Strom, A. M.; Tadayon, S. N.; Lehman, B. P.; Zirbes, A. M.; Bhattacharyya, S.; Musier-Forsyth, K.; Hati, S., Multiple Pathways Promote Dynamical Coupling between Catalytic Domains in Escherichia coli Prolyl-tRNA Synthetase. *Biochemistry* **2013,** *52* (25), 4399-4412.

196. Copeland, K. L.; Pellock, S. J.; Cox, J. R.; Cafiero, M. L.; Tschumper, G. S., Examination of Tyrosine/Adenine Stacking Interactions in Protein Complexes. *J. Phys. Chem. B* **2013,** *117* (45), 14001-14008.

197. DiGiovanni, K. M.; Hatstat, A. K.; Rote, J.; Cafiero, M., MP2//DFT calculations of interaction energies between acetaminophen and acetaminophen analogues and the aryl sulfotransferase active site. *Comput. Theor. Chem.* **2013,** *1007*, 41-47.

198. Bustos, D. J.; Temelso, B.; Shields, G. C., Hydration of the Sulfuric Acid-Methylamine Complex and Implications for Aerosol Formation. *J. Phys. Chem. A* **2014,** *118* (35), 7430-7441.

199. Pérez, C.; Zaleski, D. P.; Seifert, N. A.; Temelso, B.; Shields, G. C.; Kisiel, Z.; Pate, B. H., Hydrogen Bond Cooperativity and the Three-Dimensional Structures of Water Nonamers and Decamers. *Angew Chem Int Ed Engl* **2014,** *53* (52), 14368-14372.

200. Temelso, B.; Alser, K. A.; Gauthier, A.; Palmer, A. K.; Shields, G. C., Structural Analysis of alpha-Fetoprotein (AFP)-like Peptides with Anti-Breast-Cancer Properties. *J. Phys. Chem. B* **2014,** *118* (17), 4514-4526.

201. Wenzel, S.; Nemec, H.; Anderson, K. E.; Siepmann, J. I., Monte Carlo Simulations of Thin Hydrocarbon Films: Composition Heterogeneity and Structure at the Solid-Liquid and Liquid-Vapor Interfaces. *Langmuir* **2014,** *30* (11), 3086-3094.

202. Nguyen, P. H.; West, H.; Feske, B. D.; Padgett, C. W., Enantioselectivity and Enzyme-Substrate Docking Studies of a Ketoreductase from Sporobolomyces salmonicolor (SSCR) and Saccharomyces cerevisiae (YOL151w). *International Scholarly Research Notices* **2014,** *12428*.

203. Whiteside, T. S.; Priest, M. A.; Padgett, C. W., Modeling the interfacial thermal resistance of diamond nanorod composites and related materials. *International Journal of Computational Materials Science and Engineering* **2014,** *3* (3), 1450014-1.

204. Bartholow, T. G.; Sanford, B. L.; Cao, B.; Schmit, H. L.; Johnson, J. M.; Meitzner, J.; Bhattacharyya, S.; Musier-Forsyth, K.; Hati, S., Strictly Conserved Lysine of Prolyl-tRNA Synthetase Editing Domain Facilitates Binding and Positioning of Misacylated tRNA(Pro). *Biochemistry* **2014,** *53* (6), 1059-1068.

205. Strom, A. M.; Fehling, S. C.; Bhattacharyya, S.; Hati, S., Probing the global and local dynamics of aminoacyl-tRNA synthetases using all-atom and coarse-grained simulations. *Journal of Molecular Modeling* **2014,** *20* (5).

206. Gao, D.; Lang, D.; Robinson, T., Computational study of the thermodynamic stabilities of hydrogen-bonded complexes in solution. *Theoretical Chemistry Accounts* **2014,** *133* (11).

207. Tlach, B. C.; Tomlinson, A. L.; Morgan, K. D.; Collins, C. R.; Zenner, M. D.; Jeffries-El, M., Effect of Extended Conjugation on the Optoelectronic Properties of Benzo 1,2-d:4,5-d' bisoxazole Polymers. *Australian Journal of Chemistry* **2014,** *67* (5), 711-721.

208. Cervantes-Navarro, F.; Martinez-Guajardo, G.; Osorio, E.; Moreno, D.; Tiznado, W.; Islas, R.; Donald, K. J.; Merino, G., Stop rotating! One substitution halts the B-19(-) motor. *Chemical Communications* **2014,** *50* (73), 10680-10682.

209. Kanters, R. P. F.; Donald, K. J., CLUSTER: Searching for Unique Low Energy Minima of Structures Using a Novel Implementation of a Genetic Algorithm. *J. Chem. Theory Comput.* **2014,** *10* (12), 5729-5737.

210. Tawfik, M.; Donald, K. J., Halogen Bonding: Unifying Perspectives on Organic and Inorganic Cases. *J. Phys. Chem. A* **2014,** *118* (43), 10090-10100.

211. Helminiak, H. M.; Knauf, R. R.; Danforth, S. J.; Phillips, J. A., Structural and Energetic Properties of Acetonitrile-Group IV (A & B) Halide Complexes. *J. Phys. Chem. A* **2014,** *118* (24), 4266-4277.

212. Murdachaew, G.; Varner, M. E.; van der Veer, W. E.; Gerber, R. B.; Phillips, L. F., Raman spectroscopy of solutions and interfaces containing nitrogen dioxide, water, and 1,4 dioxane: Evidence for repulsion of surface water by NO2 gas. *J. Chem. Phys.* **2014,** *140* (18).

213. Wrass, J. P.; Sadowsky, D.; Bloomgren, K. M.; Cramer, C. J.; Phillips, J. A., Quantum chemical and matrix-IR characterization of CH3CN-BCl3: a complex with two distinct minima along the B-N bond potential. *Phys. Chem. Chem. Phys.* **2014,** *16* (31), 16480-16491.

214. Kohrt, D.; Crary, J.; Zimmer, M.; Patrick, A. N.; Ford, H. L.; Hinds, P. W.; Grossel, M. J., CDK6 binds and promotes the degradation of the EYA2 protein. *Cell Cycle* **2014,** *13* (1), 62-71.

215. Zimmer, M. H.; Li, B.; Shahid, R.; Peshkepija, P.; Zimmer, M., Structural consequences of chromophore formation and exploration of conserved lid residues amongst naturally occurring fluorescent proteins. *Chemical Physics* **2014,** *429*, 5-11.

216. Eggimann, B. L.; Sunnarborg, A. J.; Stern, H. D.; Bliss, A. P.; Siepmann, J. I., An online parameter and property database for the TraPPE force field. *Molecular Simulation* **2014,** *40* (1-3), 101-105.

217. Miller, B. R., III; Parish, C. A.; Wu, E. Y., Molecular Dynamics Study of the Opening Mechanism for DNA Polymerase I. *Plos Computational Biology* **2014,** *10* (12).

218. Miller, B. R., III; Beese, L. S.; Parish, C. A.; Wu, E. Y., The Closing Mechanism of DNA Polymerase I at Atomic Resolution. *Structure* **2015,** *23* (9), 1609-1620.

219. Muya, J. T.; Ceulemans, A.; Gopakumar, G.; Parish, C. A., Jahn-Teller Distortion in Polyoligomeric Silsesquioxane (POSS) Cations. *J. Phys. Chem. A* **2015,** *119* (18), 4237-4243.

220. Wu, E. Y.; Walsh, A. R.; Materne, E. C.; Hiltner, E. P.; Zielinski, B.; Miller, B. R., III; Mawby, L.; Modeste, E.; Parish, C. A.; Barnes, W. M.; Kermekchiev, M. B., A Conservative lsoleucine to Leucine Mutation Causes Major Rearrangements and Cold Sensitivity in KlenTaq1 DNA Polymerase. *Biochemistry* **2015,** *54* (3), 881-889.

221. Seybold, P. G.; Shields, G. C., Computational estimation of pK(a) values. *Wiley Interdisciplinary Reviews-Computational Molecular Science* **2015,** *5* (3), 290-297.

222. Swan, J. S.; Findeis, P. M.; Hilton, S.; Lebold, K. M.; Temelso, B.; Shields, G. C., Formation of deprotonated 2-imidazoline-4(5)-one product ions in the collision-induced dissociation of some serine-containing dipeptides. *International Journal of Mass Spectrometry* **2015,** *381*, 25-32.

223. Temelso, B.; Renner, C. R.; Shields, G. C., Importance and Reliability of Small Basis Set CCSD(T) Corrections to MP2 Binding and Relative Energies of Water Clusters. *J. Chem. Theory Comput.* **2015,** *11* (4), 1439-1448.

224. Lynch, W. E.; Padgett, C. W.; Quillian, B.; Haddock, J., A square-planar hydrated cationic tetrakis(methimazole)gold(III) complex. *Acta Crystallographica Section C-Structural Chemistry* **2015,** *71*, 298-+.

225. Baird, W. H.; Padgett, C. W.; Secrest, J. A., Google Earth (Science). *Physics Education* **2015,** *50*.

226. Ghosh, D.; Rhodes, S.; Hawkins, K.; Winder, D.; Atkinson, A.; Ming, W.; Padgett, C.; Orvis, J.; Aiken, K.; Landge, S., A simple and effective 1,2,3-triazole based "turn-on" fluorescence sensor for the detection of anions. *New Journal of Chemistry* **2015,** *39* (1), 295-303.

227. Quillian, B.; Hendricks, J.; Trivitayakhun, M.; Padgett, C. W., Isolation of 3-amino-4-nitro-benzyl acetate: evidence of an undisclosed impurity in 5-amino-2-nitro-benzoic acid. *Acta crystallographica. Section E, Crystallographic communications* **2015,** *71* (Pt 6), 606-8.

228. Bigler, D. J.; Peterson, L. W.; Cafiero, M., DFT and MP2 study of the effects of mutations on the binding of ligands within the SULT1A3 active site. *Comput. Theor. Chem.* **2015,** *1068*, 63-71.

229. Bigler, D. J.; Peterson, L. W.; Cafiero, M., Effects of implicit solvent and relaxed amino acid side chains on the MP2 and DFT calculations of ligand-protein structure and electronic interaction energies of dopaminergic ligands in the SULT1A3 enzyme active site. *Comput. Theor. Chem.* **2015,** *1051*, 79-92.

230. Bresnahan, C. G.; Reinhardt, C. R.; Bartholow, T. G.; Rumpel, J. P.; North, M.; Bhattacharyya, S., Effect of Stacking Interactions on the Thermodynamics and Kinetics of Lumiflavin: A Study with Improved Density Functionals and Density Functional Tight-Binding Protocol. *J. Phys. Chem. A* **2015,** *119* (1), 172-182.

231. Donald, K. J.; Kretz, W. J.; Omorodion, O., The HgF2 Ionic Switch: A Triumph of Electrostatics against Relativistic Odds. *Chem.-Eur. J.* **2015,** *21* (47), 16848-16858.

232. Donald, K. J.; Stewart, J.; Guarino, M., Structure, bonding, relativistic effects, and dispersion in the group 12 dihalide (MX2)(3) clusters, with lessons from the extended solids. *Structural Chemistry* **2015,** *26* (5-6), 1179-1195.

233. Donald, K. J.; Tawfik, M.; Buncher, B., Weak Interactions as Diagnostic Tools for Inductive Effects. *J. Phys. Chem. A* **2015,** *119* (16), 3780-3788.

234. Shao, Y.; Gan, Z.; Epifanovsky, E.; Gilbert, A. T. B.; Wormit, M.; Kussmann, J.; Lange, A. W.; Behn, A.; Deng, J.; Feng, X.; Ghosh, D.; Goldey, M.; Horn, P. R.; Jacobson, L. D.; Kaliman, I.; Khaliullin, R. Z.; Kus, T.; Landau, A.; Liu, J.; Proynov, E. I.; Rhee, Y. M.; Richard, R. M.; Rohrdanz, M. A.; Steele, R. P.; Sundstrom, E. J.; Woodcock, H. L., III; Zimmerman, P. M.; Zuev, D.; Albrecht, B.; Alguire, E.; Austin, B.; Beran, G. J. O.; Bernard, Y. A.; Berquist, E.; Brandhorst, K.; Bravaya, K. B.; Brown, S. T.; Casanova, D.; Chang, C.-M.; Chen, Y.; Chien, S. H.; Closser, K. D.; Crittenden, D. L.; Diedenhofen, M.; DiStasio, R. A., Jr.; Do, H.; Dutoi, A. D.; Edgar, R. G.; Fatehi, S.; Fusti-Molnar, L.; Ghysels, A.; Golubeva-Zadorozhnaya, A.; Gomes, J.; Hanson-Heine, M. W. D.; Harbach, P. H. P.; Hauser, A. W.; Hohenstein, E. G.; Holden, Z. C.; Jagau, T.-C.; Ji, H.; Kaduk, B.; Khistyaev, K.; Kim, J.; Kim, J.; King, R. A.; Klunzinger, P.; Kosenkov, D.; Kowalczyk, T.; Krauter, C. M.; Lao, K. U.; Laurent, A. D.; Lawler, K. V.; Levchenko, S. V.; Lin, C. Y.; Liu, F.; Livshits, E.; Lochan, R. C.; Luenser, A.; Manohar, P.; Manzer, S. F.; Mao, S.-P.; Mardirossian, N.; Marenich, A. V.; Maurer, S. A.; Mayhall, N. J.; Neuscamman, E.; Oana, C. M.; Olivares-Amaya, R.; O'Neill, D. P.; Parkhill, J. A.; Perrine, T. M.; Peverati, R.; Prociuk, A.; Rehn, D. R.; Rosta, E.; Russ, N. J.; Sharada, S. M.; Sharma, S.; Small, D. W.; Sodt, A.; Stein, T.; Stueck, D.; Su, Y.-C.; Thom, A. J. W.; Tsuchimochi, T.; Vanovschi, V.; Vogt, L.; Vydrov, O.; Wang, T.; Watson, M. A.; Wenzel, J.; White, A.; Williams, C. F.; Yang, J.; Yeganeh, S.; Yost, S. R.; You, Z.-Q.; Zhang, I. Y.; Zhang, X.; Zhao, Y.; Brooks, B. R.; Chan, G. K. L.; Chipman, D. M.; Cramer, C. J.; Goddard, W. A., III; Gordon, M. S.; Hehre, W. J.; Klamt, A.; Schaefer, H. F., III; Schmidt, M. W.; Sherrill, C. D.; Truhlar, D. G.; Warshel, A.; Xu, X.; Aspuru-Guzik, A.; Baer, R.; Bell, A. T.; Besley, N. A.; Chai, J.-D.; Dreuw, A.; Dunietz, B. D.; Furlani, T. R.; Gwaltney, S. R.; Hsu, C.-P.; Jung, Y.; Kong, J.; Lambrecht, D. S.; Liang, W.; Ochsenfeld, C.; Rassolov, V. A.; Slipchenko, L. V.; Subotnik, J. E.; Van Voorhis, T.; Herbert, J. M.; Krylov, A. I.; Gill, P. M. W.; Head-Gordon, M., Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics* **2015,** *113* (2), 184-215.

235. Flores, S. D. P.; Martin-Noble, G. C.; Phillips, R. L.; Schrier, J., Bio-Inspired Electroactive Organic Molecules for Aqueous Redox Flow Batteries. 1. Thiophenoquinones. *Journal of Physical Chemistry C* **2015,** *119* (38), 21800-21809.

236. Krueger, R. A.; Haibach, F. G.; Fry, D. L.; Gomez, M. A., Centrality measures highlight proton traps and access points to proton highways in kinetic Monte Carlo trajectories. *J. Chem. Phys.* **2015,** *142* (15).

237. Nguyen, A. H.; Koc, M. A.; Shepherd, T. D.; Molinero, V., Structure of the Ice-Clathrate Interface. *Journal of Physical Chemistry C* **2015,** *119* (8), 4104-4117.

238. Schrier, J., *Introduction to Computational Physical Chemistry*. University Science Books: Mill Valley, CA, 2017.

239. Shields, G. C.; Seybold, P. G., *Computational approaches for the prediction of pKa values*. Paperback ed.; CRC Press: 2017.

240. Navea, J. G.; Grassian, V. H., Photochemistry of atmospheric particles. In *Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry*, Wandelt, K., Kolasinski, K., Ed. Elsevier: Amsterdam, 2017.

241. Shields, G. C.; Gajdosik-Nivens, D. A.; Ness, T., Using Early Introduction to Research To Increase STEM Majors: A Tale of Two Colleges, One Small Highly Selective Private and One Non-Selective Regional Public. In *Educational and Outreach Projects from the Cottrell Scholars Collaborative: Undergraduate and Graduate Education, Vol 1*, Waterman, R.; Feig, A., Eds. 2017; Vol. 1248, pp 107-119.

242. Rovnyak, D.; Shields, G. C., A Roadmap to Successful Collaborations between Primarily Undergraduate Institutions and Research Institutions. In *Credit Where Credit Is Due: Respecting Authorship and Intellectual Property*, Mabrouk, P. A.; Currano, J. N., Eds. 2018; Vol. 1291, pp 105-127.

243. Hati, S.; Bhattacharyya, S., Integrating Research into the Curriculum: A Low-Cost Strategy for Promoting Undergraduate Research. In *Best Practices for Supporting and Expanding Undergraduate Research in Chemistry*, American Chemical Society: 2018; Vol. 1275, pp 119-141.

244. Carter, L. C.; Foss, K. M.; Mohler, D. L.; Wilson, D. L.; Sumner, I., Forming Bonds: Using Community Outreach To Maintain Relationships with Other Chemistry Societies. In *Building and Maintaining Award-Winning ACS Student Member Chapters Volume 3*, American Chemical Society: 2018; Vol. 1278, pp 27-37.

245. Bruce, C. D., Molecular Dynamics Simulations in First-Semester General Chemistry: Visualizing Gas Particle Motion and Making Connections to Mathematical Gas Law Relationships. In *Using Computational Methods To Teach Chemical Principles*, American Chemical Society: 2019; Vol. 1312, pp 11-19.

246. Phillips, J. A., Modeling Reaction Energies and Exploring Noble Gas Chemistry in the Physical Chemistry Laboratory. In *Using Computational Methods To Teach Chemical Principles*, American Chemical Society: 2019; Vol. 1312, pp 33-50.

247. McDonald, A. R.; Hagen, J. P., Beyond the Analytical Solution: Using Mathematical Software To Enhance Understanding of Physical Chemistry. In *Using Computational Methods To Teach Chemical Principles*, American Chemical Society: 2019; Vol. 1312, pp 195-210.

248. Kholod, Y.; Kosenkov, D., Discovery-Based Computational Activities in the Undergraduate Chemistry Curriculum. In *Using Computational Methods To Teach Chemical Principles*, American Chemical Society: 2019; Vol. 1312, pp 227-243.

249. Adler, P. D. F.; Xu, R. J.; Olshansky, J. H.; Smith, M. D.; Elbert, K. C.; Yang, Y.; Ferrence, G. M.; Zeller, M.; Schrier, J.; Norquist, A. J., Probing structural adaptability in templated vanadium selenites. *Polyhedron* **2016,** *114*, 184-193.

250. Baker, J. L.; Jafri, H., Molecular simulations of lactose-bound and unbound forms of the FaeG adhesin reveal critical amino acids involved in sugar binding. *Journal of Molecular Graphics and Modelling* **2016,** *70*, 100-108.

251. Ball, K. A.; Johnson, J. R.; Lewinski, M. K.; Guatelli, J.; Verschueren, E.; Krogan, N. J.; Jacobson, M. P., Non-degradative Ubiquitination of Protein Kinases. *PLOS Computational Biology* **2016,** *12* (6), e1004898.

252. Baltrusaitis, J.; Patterson, E. V.; O’Connor, M.; Qu, S.; Kolodziej, E. P.; Cwiertny, D. M., Reversible Photohydration of Trenbolone Acetate Metabolites: Mechanistic Understanding of Product-to-Parent Reversion through Complementary Experimental and Theoretical Approaches. *Environmental Science & Technology* **2016,** *50* (13), 6753-6761.

253. Borgatta, J.; Paskavitz, A.; Kim, D.; Navea, J. G., Comparative evaluation of iron leach from different sources of fly ash under atmospherically relevant conditions. *Environmental Chemistry* **2016,** *13* (5), 902-912.

254. Chavez, I., Ramiro; Cai, M.; Tlach, B.; Wheeler, D. L.; Kaudal, R.; Tsyrenova, A.; Tomlinson, A. L.; Shinar, R.; Shinar, J.; Jeffries-EL, M., Benzobisoxazole cruciforms: A tunable, cross-conjugated platform for the generation of deep blue OLED materials. *Journal of Materials Chemistry C* **2016**, Medium: ED; Size: p. 3765-3773.

255. Chen, H.; Varner, M. E.; Gerber, R. B.; Finlayson-Pitts, B. J., Reactions of Methanesulfonic Acid with Amines and Ammonia as a Source of New Particles in Air. *The Journal of Physical Chemistry B* **2016,** *120* (8), 1526-1536.

256. Du Pont, K. E.; McKenzie, A. M.; Kokhan, O.; Sumner, I.; Berndsen, C. E., The Disulfide Bonds within BST-2 Enhance Tensile Strength during Viral Tethering. *Biochemistry* **2016,** *55* (6), 940-947.

257. Famularo, N.; Kholod, Y.; Kosenkov, D., Integrating Chemistry Laboratory Instrumentation into the Industrial Internet: Building, Programming, and Experimenting with an Automatic Titrator. *Journal of Chemical Education* **2016,** *93* (1), 175-181.

258. Gomez, M. A.; Fry, D. L.; Sweet, M. E., Effects on the Proton Conduction Limiting Barriers and Trajectories in BaZr0.875Y0.125O3 Due to the Presence of Other Protons. *Journal of the Korean Ceramic Society* **2016,** *53* (5), 521-528.

259. Gurunathan, P. K.; Acharya, A.; Ghosh, D.; Kosenkov, D.; Kaliman, I.; Shao, Y.; Krylov, A. I.; Slipchenko, L. V., Extension of the Effective Fragment Potential Method to Macromolecules. *The Journal of Physical Chemistry B* **2016,** *120* (27), 6562-6574.

260. Hatstat, A. K.; Morris, M.; Peterson, L. W.; Cafiero, M., Ab initio study of electronic interaction energies and desolvation energies for dopaminergic ligands in the catechol-O-methyltransferase active site. *Comput. Theor. Chem.* **2016,** *1078*, 146-162.

261. Hocky, G. M.; Baker, J. L.; Bradley, M. J.; Sinitskiy, A. V.; De La Cruz, E. M.; Voth, G. A., Cations Stiffen Actin Filaments by Adhering a Key Structural Element to Adjacent Subunits. *The Journal of Physical Chemistry B* **2016,** *120* (20), 4558-4567.

262. Homayoon, Z.; Pratihar, S.; Dratz, E.; Snider, R.; Spezia, R.; Barnes, G. L.; Macaluso, V.; Martin Somer, A.; Hase, W. L., Model Simulations of the Thermal Dissociation of the TIK(H+)2 Tripeptide: Mechanisms and Kinetic Parameters. *The Journal of Physical Chemistry A* **2016,** *120* (42), 8211-8227.

263. Jalife, S.; Liu, L.; Pan, S.; Cabellos, J. L.; Osorio, E.; Lu, C.; Heine, T.; Donald, K. J.; Merino, G., Dynamical behavior of boron clusters. *Nanoscale* **2016,** *8* (40), 17639-17644.

264. Kosenkov, D., PyFREC: Software for Förster electronic coupling evaluation in molecular fragments. *Journal of Computational Chemistry* **2016,** *37* (19), 1847-1854.

265. Kosenkov, D.; Shaw, J.; Zuczek, J.; Kholod, Y., Transient-Absorption Spectroscopy of Cis–Trans Isomerization of N,N-Dimethyl-4,4′-azodianiline with 3D-Printed Temperature-Controlled Sample Holder. *Journal of Chemical Education* **2016,** *93* (7), 1299-1304.

266. Nourmahnad, A.; Wenny, M. B.; Zeller, M.; Schrier, J.; Norquist, A. J., The role of inorganic acidity on templated vanadate composition and dimensionality. *Journal of Solid State Chemistry* **2016,** *236*, 215-221.

267. Omorodion, O.; Bober, M.; Donald, K. J., Turn: Weak Interactions and Rotational Barriers in Molecules—Insights from Substituted Butynes. *The Journal of Physical Chemistry A* **2016,** *120* (44), 8896-8906.

268. Phillips, J. A., Structural and energetic properties of nitrile–BX3 complexes: substituent effects and their impact on condensed-phase sensitivity. *Theoretical Chemistry Accounts* **2016,** *136* (1), 16.

269. Pratihar, S.; Barnes, G. L.; Hase, W. L., Chemical dynamics simulations of energy transfer, surface-induced dissociation, soft-landing, and reactive-landing in collisions of protonated peptide ions with organic surfaces. *Chem. Soc. Rev.* **2016,** *45* (13), 3595-3608.

270. Pratihar, S.; Barnes, G. L.; Laskin, J.; Hase, W. L., Dynamics of Protonated Peptide Ion Collisions with Organic Surfaces: Consonance of Simulation and Experiment. *The Journal of Physical Chemistry Letters* **2016,** *7* (16), 3142-3150.

271. Raccuglia, P.; Elbert, K. C.; Adler, P. D. F.; Falk, C.; Wenny, M. B.; Mollo, A.; Zeller, M.; Friedler, S. A.; Schrier, J.; Norquist, A. J., Machine-learning-assisted materials discovery using failed experiments. *Nature* **2016,** *533* (7601), 73-76.

272. Richardson, J. O.; Perez, C.; Lobsiger, S.; Reid, A. A.; Temelso, B.; Shields, G. C.; Kisiel, Z.; Wales, D. J.; Pate, B. H.; Althorpe, S. C., Concerted hydrogen-bond breaking by quantum tunneling in the water hexamer prism. *Science* **2016,** *351* (6279), 1310-1313.

273. Weiss, N. M.; Waller, A. W.; Phillips, J. A., Infrared spectrum of CH3CN–HCl in solid neon, and modeling matrix effects in CH3CN–HCl and H3N–HCl. *Journal of Molecular Structure* **2016,** *1105*, 341-349.

274. Beane, A.; Miller, B. R.; Parish, C. A., Internal abstraction of dynemicin A: An MD approach. *Journal of Molecular Graphics and Modelling* **2017,** *74*, 251-264.

275. Barnes, G. L.; Podczerwinski, A., Simulating the Effect of Charge State on Reactive Landing of a Cyclic Tetrapeptide on Chemically Modified Alkylthiolate Self-Assembled Monolayer Surfaces. *The Journal of Physical Chemistry C* **2017,** *121* (27), 14628-14635.

276. Bunn, H.; Soliday, R. M.; Sumner, I.; Raston, P. L., Far-infrared Spectroscopic Characterization ofAnti-vinyl Alcohol. *The Astrophysical Journal* **2017,** *847* (1), 67.

277. Chaudhuri, S.; Hedstrom, S.; Mendez-Hernandez, D. D.; Hendrickson, H. P.; Jung, K. A.; Ho, J. M.; Batista, V. S., Electron Transfer Assisted by Vibronic Coupling from Multiple Modes. *J. Chem. Theory Comput.* **2017,** *13* (12), 6000-6009.

278. Donald, K. J.; Befekadu, E.; Prasad, S., Coordination and Insertion: Competitive Channels for Borylene Reactions. *J. Phys. Chem. A* **2017,** *121* (46), 8982-8994.

279. Gomez, M. A.; Kwan, G.; Zhu, W.; Chelliah, M.; Zuo, X.; Eshun, A.; Blackmer, V.; Huynh, T.; Huynh, M., Ordered yttrium concentration effects on barium zirconate structure, proton binding sites and transition states. *Solid State Ionics* **2017,** *304*, 126-134.

280. Guo, Y.; Hendrickson, H. P.; Videla, P. E.; Chen, Y.-N.; Ho, J.; Sekharan, S.; Batista, V. S.; Tully, J. C.; Yan, E. C. Y., Probing the remarkable thermal kinetics of visual rhodopsin with E181Q and S186A mutants. *The Journal of Chemical Physics* **2017,** *146* (21), 215104.

281. Heyert, A. J.; Knox, S. L.; Lindberg, G. E.; Baker, J. L., Influence of an ionic liquid on the conformational sampling of Xaa-Pro dipeptides. *Journal of Molecular Liquids* **2017,** *227*, 66-75.

282. Jafari, M.; Welden, A. R.; Williams, K. L.; Winograd, B.; Mulvihill, E.; Hendrickson, H. P.; Lenard, M.; Gottfried, A.; Geva, E., Compute-to-Learn: Authentic Learning via Development of Interactive Computer Demonstrations within a Peer-Led Studio Environment. *Journal of Chemical Education* **2017,** *94* (12), 1896-1903.

283. Kacar, B.; Hanson-Smith, V.; Adam, Z. R.; Boekelheide, N., Constraining the timing of the Great Oxidation Event within the Rubisco phylogenetic tree. *Geobiology* **2017,** *15* (5), 628-640.

284. Lipchock, J. M.; Hendrickson, H. P.; Douglas, B. B.; Bird, K. E.; Ginther, P. S.; Rivalta, I.; Ten, N. S.; Batista, V. S.; Loria, J. P., Characterization of Protein Tyrosine Phosphatase 1B Inhibition by Chlorogenic Acid and Cichoric Acid. *Biochemistry* **2017,** *56* (1), 96-106.

285. Malkowski, S. N.; Dishuck, C. F.; Lamanilao, G. G.; Embry, C. P.; Grubb, C. S.; Cafiero, M.; Peterson, L. W., Design, Modeling and Synthesis of 1,2,3-Triazole-Linked Nucleoside-Amino Acid Conjugates as Potential Antibacterial Agents. *Molecules* **2017,** *22* (10).

286. Navea, J. G.; Richmond, E.; Stortini, T.; Greenspan, J., Water Adsorption Isotherms on Fly Ash from Several Sources. *Langmuir* **2017,** *33* (39), 10161-10171.

287. Perez, C.; Steber, A. L.; Rijs, A. M.; Temelso, B.; Shields, G. C.; Lopez, J. C.; Kisiel, Z.; Schnell, M., Corannulene and its complex with water: a tiny cup of water. *Phys. Chem. Chem. Phys.* **2017,** *19* (22), 14214-14223.

288. Phillips, J. A.; Danforth, S. J.; Hora, N. J.; Lanska, J. R.; Waller, A. W., Structural and Energetic Properties of Haloacetonitrile–BCl3 Complexes: Computations and Matrix-IR Spectroscopy. *The Journal of Physical Chemistry A* **2017,** *121* (48), 9252-9261.

289. Pratihar, S.; Ma, X.; Homayoon, Z.; Barnes, G. L.; Hase, W. L., Direct Chemical Dynamics Simulations. *Journal of the American Chemical Society* **2017,** *139* (10), 3570-3590.

290. Carro, J.; Martinez-Julvez, M.; Medina, M.; Martinez, A. T.; Ferreira, P., Protein dynamics promote hydride tunnelling in substrate oxidation by aryl-alcohol oxidase. *Phys. Chem. Chem. Phys.* **2017,** *19* (42), 28666-28675.

291. Saha, I.; Wang, E. B.; Parish, C. A.; Ghosh, K., Triphenylamine-Based Open and Macrocyclic Receptors: A Study Towards Selectivite Recognition of Aliphatic Dicarboxylates. *ChemistrySelect* **2017,** *2* (17), 4794-4799.

292. Sarkar, S.; Hendrickson, H. P.; Lee, D.; DeVine, F.; Jung, J.; Geva, E.; Kim, J.; Dunietz, B. D., Phosphorescence in Bromobenzaldehyde Can Be Enhanced through Intramolecular Heavy Atom Effect. *The Journal of Physical Chemistry C* **2017,** *121* (7), 3771-3777.

293. Steber, A. L.; Perez, C.; Temelso, B.; Shields, G. C.; Rijs, A. M.; Pate, B. H.; Kisiel, Z.; Schnell, M., Capturing the Elusive Water Trimer from the Stepwise Growth of Water on the Surface of the Polycyclic Aromatic Hydrocarbon Acenaphthene. *Journal of Physical Chemistry Letters* **2017,** *8* (23), 5744-5750.

294. Taylor, C. A.; Miller, B. R.; Parish, C. A., Design and computational support for the binding stability of a new CCR5/CXCR4 dual tropic inhibitor: Computational design of a CCR5/CXCR4 drug. *Journal of Molecular Graphics and Modelling* **2017,** *75*, 71-79.

295. Taylor, C. A.; Miller III, B. R.; Shah, S. S.; Parish, C. A., A molecular dynamics study of the binary complexes of APP, JIP1, and the cargo binding domain of KLC. *Proteins: Structure, Function, and Bioinformatics* **2017,** *85* (2), 221-234.

296. Temelso, B.; Mabey, J. M.; Kubota, T.; Appiah-Padi, N.; Shields, G. C., ArbAlign: A Tool for Optimal Alignment of Arbitrarily Ordered Isomers Using the Kuhn-Munkres Algorithm. *Journal of Chemical Information and Modeling* **2017,** *57* (5), 1045-1054.

297. Vasiliou, A. K.; Hu, H.; Cowell, T. W.; Whitman, J. C.; Porterfield, J.; Parish, C. A., Modeling Oil Shale Pyrolysis: High-Temperature Unimolecular Decomposition Pathways for Thiophene. *The Journal of Physical Chemistry A* **2017,** *121* (40), 7655-7666.

298. Waller, A. W.; Weiss, N. M.; Decato, D. A.; Phillips, J. A., Structural and energetic properties of haloacetonitrile - GeF4 complexes. *Journal of Molecular Structure* **2017,** *1130*, 984-993.

299. Wang, W.; Taylor, C.; Hu, H.; Humphries, K. L.; Jaini, A.; Kitimet, M.; Scott, T.; Stewart, Z.; Ulep, K. J.; Houck, S.; Luxon, A.; Zhang, B.; Miller, B.; Parish, C. A.; Pomerantz, A. E.; Mullins, O. C.; Zare, R. N., Nanoaggregates of Diverse Asphaltenes by Mass Spectrometry and Molecular Dynamics. *Energy & Fuels* **2017,** *31* (9), 9140-9151.

300. Wheeler, D. L.; Rainwater, L. E.; Green, A. R.; Tomlinson, A. L., Modeling electrochromic poly-dioxythiophene-containing materials through TDDFT. *Phys. Chem. Chem. Phys.* **2017,** *19* (30), 20251-20258.

301. Wilson, R. H.; Zamfir, S.; Sumner, I., Molecular dynamics simulations reveal a new role for a conserved active site asparagine in a ubiquitin-conjugating enzyme. *Journal of Molecular Graphics and Modelling* **2017,** *76*, 403-411.

302. Yao, B.; Mandrà, S.; Curry, J. O.; Shaikhutdinov, S.; Freund, H.-J.; Schrier, J., Gas Separation through Bilayer Silica, the Thinnest Possible Silica Membrane. *ACS Applied Materials & Interfaces* **2017,** *9* (49), 43061-43071.

303. Yeager, A. V.; Swails, J. M.; Miller, B. R., Improved Accuracy for Constant pH-REMD Simulations through Modification of Carboxylate Effective Radii. *J. Chem. Theory Comput.* **2017,** *13* (10), 4624-4635.

304. Christiansen, D. T.; Wheeler, D. L.; Tomlinson, A. L.; Reynolds, J. R., Electrochromism of alkylene-linked discrete chromophore polymers with broad radical cation light absorption. *Polymer Chemistry* **2018,** *9* (22), 3055-3066.

305. Dewar, J. C.; Thakur, A. S.; Brennessel, W. W.; Cafiero, M.; Peterson, L. W.; Eckenhoff, W. T., Simple zinc complex to model substrate binding to zinc enzymes. *Inorganica Chimica Acta* **2018,** *473*, 15-19.

306. Dong, J. J.; Klumpp, S., Simulation of colony pattern formation under differential adhesion and cell proliferation. *Soft Matter* **2018,** *14* (10), 1908-1916.

307. Esseffar, M. h.; Parish, C. A.; Jalal, R.; Lamsabhi, A. M., A Computational Study of the Reactivity of 3,5-(Oxo/Thioxo) Derivatives of 2,7-Dimethyl-1,2,4-Triazepines. Keto–Enol Tautomerization and Potential for Hydrogen Storage. *The Journal of Physical Chemistry A* **2018,** *122* (11), 3076-3086.

308. Evans, R.; Peterson, L.; Cafiero, M., Evaluation of hybrid and pure DFT methods for the binding of novel ligands in the tyrosine hydroxylase enzyme. *Comput. Theor. Chem.* **2018,** *1140*, 145-151.

309. Frederickson, D.; McDonough, M.; Barnes, G. L., A Computational Comparison of Soft Landing of α-Helical vs Globular Peptides. *The Journal of Physical Chemistry B* **2018,** *122* (41), 9549-9554.

310. Hora, N. J.; Wahl, B. M.; Soares, C.; Lara, S. A.; Lanska, J. R.; Phillips, J. A., On the interactions of nitriles and fluoro-substituted pyridines with silicon tetrafluoride: Computations and thin film IR spectroscopy. *Journal of Molecular Structure* **2018,** *1157*, 679-692.

311. Hu, H.; Zhang, B.; Luxon, A.; Scott, T.; Wang, B.; Parish, C. A., An Extended Multireference Study of the Singlet and Triplet States of the 9,10-didehydroanthracene Diradical. *The Journal of Physical Chemistry A* **2018,** *122* (14), 3688-3696.

312. Hunter, N. H.; Bakula, B. C.; Bruce, C. D., Molecular dynamics simulations of apo and holo forms of fatty acid binding protein 5 and cellular retinoic acid binding protein II reveal highly mobile protein, retinoic acid ligand, and water molecules. *Journal of Biomolecular Structure and Dynamics* **2018,** *36* (7), 1893-1907.

313. Kholod, Y.; Hoag, E.; Muratore, K.; Kosenkov, D., Computer-Aided Drug Discovery: Molecular Docking of Diminazene Ligands to DNA Minor Groove. *Journal of Chemical Education* **2018,** *95* (5), 882-887.

314. Kholod, Y.; DeFilippo, M.; Reed, B.; Valdez, D.; Gillan, G.; Kosenkov, D., Excitation energy transfer pathways in light-harvesting proteins: Modeling with PyFREC. *Journal of Computational Chemistry* **2018,** *39* (8), 438-449.

315. Kumar, A.; Nguyen, A. H.; Okumu, R.; Shepherd, T. D.; Molinero, V., Could Mesophases Play a Role in the Nucleation and Polymorph Selection of Zeolites? *Journal of the American Chemical Society* **2018,** *140* (47), 16071-16086.

316. Luxon, A. R.; Orms, N.; Kanters, R.; Krylov, A. I.; Parish, C. A., An ab Initio Exploration of the Bergman Cyclization. *The Journal of Physical Chemistry A* **2018,** *122* (1), 420-430.

317. Mellis, B.; Soto, P.; Bruce, C. D.; Lacueva, G.; Wilson, A. M.; Jayasekare, R., Factors affecting the number and type of student research products for chemistry and physics students at primarily undergraduate institutions: A case study. *PLOS ONE* **2018,** *13* (4), e0196338.

318. Negre, C. F. A.; Morzan, U. N.; Hendrickson, H. P.; Pal, R.; Lisi, G. P.; Loria, J. P.; Rivalta, I.; Ho, J. M.; Batista, V. S., Eigenvector centrality for characterization of protein allosteric pathways. *Proc. Natl. Acad. Sci. U. S. A.* **2018,** *115* (52), E12201-E12208.

319. Newkirk, M. L.; Rubenstein, K. J.; Kim, J. Y.; Labrecque, C. L.; Airas, J.; Taylor, C. A.; Evans, H. D.; McKoy, Q.; Parish, C. A.; Pollock, J. A., Analysis of MEMO1 Binding Specificity for ErbB2 Using Fluorescence Polarization and Molecular Dynamics Simulations. *Biochemistry* **2018,** *57* (34), 5169-5181.

320. Ostaszewski, C. J.; Stuart, N. M.; Lesko, D. M. B.; Kim, D.; Lueckheide, M. J.; Navea, J. G., Effects of Coadsorbed Water on the Heterogeneous Photochemistry of Nitrates Adsorbed on TiO2. *The Journal of Physical Chemistry A* **2018,** *122* (31), 6360-6371.

321. Paskavitz, A. L.; Quintana, J.; Cangussu, D.; Tavera-Montañez, C.; Xiao, Y.; Ortiz-Miranda, S.; Navea, J. G.; Padilla-Benavides, T., Differential expression of zinc transporters accompanies the differentiation of C2C12 myoblasts. *Journal of Trace Elements in Medicine and Biology* **2018,** *49*, 27-34.

322. Prasad, S.; Wittmaack, B. K.; Donald, K. J., Bending Ternary Dihalides. *J. Phys. Chem. A* **2018,** *122* (46), 9065-9072.

323. Reinhardt, C. R.; Hu, Q. H.; Bresnahan, C. G.; Hati, S.; Bhattacharyya, S., Cyclic Changes in Active Site Polarization and Dynamics Drive the “Ping-pong” Kinetics in NRH:Quinone Oxidoreductase 2: An Insight from QM/MM Simulations. *ACS Catalysis* **2018,** *8* (12), 12015-12029.

324. Rodríguez, A.; Rodríguez-Fernández, R.; A. Vázquez, S.; L. Barnes, G.; J. P. Stewart, J.; Martínez-Núñez, E., tsscds2018: A code for automated discovery of chemical reaction mechanisms and solving the kinetics. *Journal of Computational Chemistry* **2018,** *39* (23), 1922-1930.

325. Shaprio, J. D.; Sonberg, J. C.; Schafer, B. C.; Williams, C. C.; Ferris, H. R.; Reinheimer, E. W.; Van Wynsberghe, A. W.; Kriley, C. E.; Majireck, M. M., Synthesis, Characterization, and Computational Modeling of N-(1-Ethoxyvinyl)pyridinium Triflates, an Unusual Class of Pyridinium Salts. *Molecules* **2018,** *23* (2).

326. Temelso, B.; Klein, K. L.; Mabey, J. W.; Perez, C.; Pate, B. H.; Kisiel, Z.; Shields, G. C., Exploring the Rich Potential Energy Surface of (H2O)(11) and Its Physical Implications. *J. Chem. Theory Comput.* **2018,** *14* (2), 1141-1153.

327. Temelso, B.; Morrison, E. F.; Speer, D. L.; Cao, B. C.; Appiah-Padi, N.; Kim, G.; Shields, G. C., Effect of Mixing Ammonia and Alkylamines on Sulfate Aerosol Formation. *J. Phys. Chem. A* **2018,** *122* (6), 1612-1622.

328. Vassilev-Galindo, V.; Pan, S.; Donald, K. J.; Merino, G., Planar pentacoordinate carbons. *Nature Reviews Chemistry* **2018,** *2* (2).

329. Wang, J.; Jeevarathinam, A. S.; Humphries, K.; Jhunjhunwala, A.; Chen, F.; Hariri, A.; Miller, B. R.; Jokerst, J. V., A Mechanistic Investigation of Methylene Blue and Heparin Interactions and Their Photoacoustic Enhancement. *Bioconjugate Chemistry* **2018,** *29* (11), 3768-3775.

330. Xu, R. J.; Olshansky, J. H.; Adler, P. D. F.; Huang, Y.; Smith, M. D.; Zeller, M.; Schrier, J.; Norquist, A. J., Understanding structural adaptability: a reactant informatics approach to experiment design. *Molecular Systems Design & Engineering* **2018,** *3* (3), 473-484.

331. Yeager, A.; Humphries, K.; Farmer, E.; Cline, G.; Miller, B. R., Investigation of Nascent Base Pair and Polymerase Behavior in the Presence of Mismatches in DNA Polymerase I Using Molecular Dynamics. *Journal of Chemical Information and Modeling* **2018,** *58* (2), 338-349.

332. Adams, L. M.; Andrews, R. J.; Hu, Q. H.; Schmit, H. L.; Hati, S.; Bhattacharyya, S., Crowder-Induced Conformational Ensemble Shift in Escherichia coli Prolyl-tRNA Synthetase. *Biophysical Journal* **2019,** *117* (7), 1269-1284.

333. Ball, K. A.; Chan, L. M.; Stanley, D. J.; Tierney, E.; Thapa, S.; Ta, H. M.; Burton, L.; Binning, J. M.; Jacobson, M. P.; Gross, J. D., Conformational Dynamics of the HIV-Vif Protein Complex. *Biophysical Journal* **2019,** *116* (8), 1432-1445.

334. Carter, E. E.; Heyert, A. J.; De Souza, M.; Baker, J. L.; Lindberg, G. E., The ionic liquid [C4mpy][Tf2N] induces bound-like structure in the intrinsically disordered protein FlgM. *Phys. Chem. Chem. Phys.* **2019,** *21* (32), 17950-17958.

335. Chavez, R.; Diodati, L.; Wheeler, D. L.; Shaw, J.; Tomlinson, A. L.; Jeffries-El, M., Evaluating the Impact of Fluorination on the Electro-optical Properties of Cross-Conjugated Benzobisoxazoles. *The Journal of Physical Chemistry A* **2019,** *123* (7), 1343-1352.

336. Christiansen, D. T.; Tomlinson, A. L.; Reynolds, J. R., New Design Paradigm for Color Control in Anodically Coloring Electrochromic Molecules. *Journal of the American Chemical Society* **2019,** *141* (9), 3859-3862.

337. Christiansen, D. T.; Ohtani, S.; Chujo, Y.; Tomlinson, A. L.; Reynolds, J. R., All Donor Electrochromic Polymers Tunable across the Visible Spectrum via Random Copolymerization. *Chemistry of Materials* **2019,** *31* (17), 6841-6849.

338. Donald, K. J.; Gillespie, S.; Shafi, Z., Ouroboros: Heterocycles closed by dative sigma bonds and stabilized by pi delocalization. *Tetrahedron* **2019,** *75* (3), 335-345.

339. Grace, D. N.; Sharp, J. R.; Holappa, R. E.; Lugos, E. N.; Sebold, M. B.; Griffith, D. R.; Hendrickson, H. P.; Galloway, M. M., Heterocyclic Product Formation in Aqueous Brown Carbon Systems. *ACS Earth and Space Chemistry* **2019,** *3* (11), 2472-2481.

340. Greene, J. R.; Merrett, K. L.; Heyert, A. J.; Simmons, L. F.; Migliori, C. M.; Vogt, K. C.; Castro, R. S.; Phillips, P. D.; Baker, J. L.; Lindberg, G. E.; Fox, D. T.; Del Sesto, R. E.; Koppisch, A. T., Scope and efficacy of the broad-spectrum topical antiseptic choline geranate. *PLOS ONE* **2019,** *14* (9), e0222211.

341. Hull, K.; Soliday, R. M.; Sumner, I.; Raston, P. L., Comment on “Revisiting the formation of cyclic clusters in liquid ethanol” [J. Chem. Phys. 144, 154302 (2016)]. *The Journal of Chemical Physics* **2019,** *150* (5), 057101.

342. Jaini, A. K. A.; Hughes, L. B.; Kitimet, M. M.; Ulep, K. J.; Leopold, M. C.; Parish, C. A., Halogen Bonding Interactions for Aromatic and Nonaromatic Explosive Detection. *ACS Sensors* **2019,** *4* (2), 389-397.

343. Jia, X.; Dixon, J. L.; Zeller, M.; Schrier, J.; Norquist, A. J., Templated vanadium tellurites: Identifying the effects of low density attractions on inorganic layer topology. *Journal of Solid State Chemistry* **2019,** *273*, 158-165.

344. Jia, X.; Lynch, A.; Huang, Y.; Danielson, M.; Lang’at, I.; Milder, A.; Ruby, A. E.; Wang, H.; Friedler, S. A.; Norquist, A. J.; Schrier, J., Anthropogenic biases in chemical reaction data hinder exploratory inorganic synthesis. *Nature* **2019,** *573* (7773), 251-255.

345. Jones, W. M.; Davis, A. G.; Wilson, R. H.; Elliott, K. L.; Sumner, I., A conserved asparagine in a ubiquitin-conjugating enzyme positions the substrate for nucleophilic attack. *Journal of Computational Chemistry* **2019,** *40* (22), 1969-1977.

346. Linden, G.; Zhang, L.; Pieck, F.; Linne, U.; Kosenkov, D.; Tonner, R.; Vázquez, O., Conditional Singlet Oxygen Generation through a Bioorthogonal DNA-targeted Tetrazine Reaction. *Angewandte Chemie International Edition* **2019,** *58* (37), 12868-12873.

347. Lindsey, R. K.; Eggimann, B. L.; Stoll, D. R.; Carr, P. W.; Schure, M. R.; Siepmann, J. I., Column selection for comprehensive two-dimensional liquid chromatography using the hydrophobic subtraction model. *Journal of Chromatography A* **2019,** *1589*, 47-55.

348. Londergan, C.; Schrier, J., Research in Physical Chemistry at Primarily Undergraduate Institutions. *The Journal of Physical Chemistry A* **2019,** *123* (15), 3239-3240.

349. Lopez, J. C.; Perez, C.; Blanco, S.; Shubert, V. A.; Temelso, B.; Shields, G. C.; Schnell, M., Water induces the same crown shapes as Li+ or Na+ in 15-crown-5 ether: a broadband rotational study. *Phys. Chem. Chem. Phys.* **2019,** *21* (6), 2875-2881.

350. Palermo, G.; Armacost, K. A.; Nagan, M. C., Women Make COMP: Mentoring the Next Generation of Women in Computational Chemistry. *Journal of Chemical Information and Modeling* **2019,** *59* (10), 4061-4062.

351. Matthews, A. D.; Prasad, S.; Schley, N. D.; Donald, K. J.; Johnson, M. W., On Transannulation in Azaphosphatranes: Synthesis and Theoretical Analysis. *Inorganic Chemistry* **2019,** *58* (23), 15983-15992.

352. Modeste, E.; Mawby, L.; Miller, B.; Wu, E.; Parish, C. A., A Molecular Dynamics Investigation of the Thermostability of Cold-Sensitive I707L KlenTaq1 DNA Polymerase and Its Wild-Type Counterpart. *Journal of Chemical Information and Modeling* **2019,** *59* (5), 2423-2431.

353. Pendleton, I. M.; Cattabriga, G.; Li, Z.; Najeeb, M. A.; Friedler, S. A.; Norquist, A. J.; Chan, E. M.; Schrier, J., Experiment Specification, Capture and Laboratory Automation Technology (ESCALATE): a software pipeline for automated chemical experimentation and data management. *MRS Communications* **2019,** *9* (3), 846-859.

354. Perchik, M. C.; Peterson, L. W.; Cafiero, M., The effects of ligand deprotonation on the binding selectivity of the phenylalanine hydroxylase active site. *Comput. Theor. Chem.* **2019,** *1153*, 19-24.

355. Pflug, N. C.; Patterson, E. V.; Martinović-Weigelt, D.; Kolodziej, E. P.; Gloer, J. B.; McNeill, K.; Cwiertny, D. M.; Wammer, K. H., Intramolecular [2 + 2] Photocycloaddition of Altrenogest: Confirmation of Product Structure, Theoretical Mechanistic Insight, and Bioactivity Assessment. *The Journal of Organic Chemistry* **2019,** *84* (17), 11366-11371.

356. Sabsay, K. R.; Lee, R. T.; Ravatt, L. M.; Oza, J. P.; McDonald, A. R., Computational Models for Activated Human MEK1: Identification of Key Active Site Residues and Interactions. *Journal of Chemical Information and Modeling* **2019,** *59* (5), 2383-2393.

357. Schmucker, D. J.; Dunbar, S. R.; Shepherd, T. D.; Bertucci, M. A., n → π\* Interactions in N-Acyl Homoserine Lactone Derivatives and Their Effects on Hydrolysis Rates. *The Journal of Physical Chemistry A* **2019,** *123* (13), 2537-2543.

358. Scott, T.; Nieman, R.; Luxon, A.; Zhang, B.; Lischka, H.; Gagliardi, L.; Parish, C. A., A Multireference Ab Initio Study of the Diradical Isomers of Pyrazine. *The Journal of Physical Chemistry A* **2019,** *123* (10), 2049-2057.

359. Gordon, S. J. V.; Xiao, Y.; Paskavitz, A. L.; Navarro-Tito, N.; Navea, J. G.; Padilla-Benavides, T., Atomic Absorbance Spectroscopy to Measure Intracellular Zinc Pools in Mammalian Cells. *JoVE* **2019,** (147), e59519.

360. Soliday, R. M.; Bunn, H.; Sumner, I.; Raston, P. L., Far-Infrared Synchrotron Spectroscopy and Quantum Chemical Calculations of the Potentially Important Interstellar Molecule, 2-Chloroethanol. *The Journal of Physical Chemistry A* **2019,** *123* (6), 1208-1216.

361. Tavera-Montañez, C.; Hainer, S. J.; Cangussu, D.; Gordon, S. J. V.; Xiao, Y.; Reyes-Gutierrez, P.; Imbalzano, A. N.; Navea, J. G.; Fazzio, T. G.; Padilla-Benavides, T., The classic metal-sensing transcription factor MTF1 promotes myogenesis in response to copper. *The FASEB Journal* **2019,** *33* (12), 14556-14574.

362. Uwimana, E.; Cagle, B.; Yeung, C.; Li, X.; Patterson, E. V.; Doorn, J. A.; Lehmler, H.-J., Atropselective Oxidation of 2,2′,3,3′,4,6′-Hexachlorobiphenyl (PCB 132) to Hydroxylated Metabolites by Human Liver Microsomes and Its Implications for PCB 132 Neurotoxicity. *Toxicological Sciences* **2019,** *171* (2), 406-420.

363. Vilchis-Nestor, A. C.; Roldán, L. M.; Leonardi, A.; Navea, J. G.; Padilla-Benavides, T.; Shoshani, L., Ouabain Enhances Cell-Cell Adhesion Mediated by β1 Subunits of the Na+,K+-ATPase in CHO Fibroblasts. *International Journal of Molecular Sciences* **2019,** *20* (9).

364. Rovnyak, D. S.; Shields, G. C., How Undergraduate Research Drives Science Forward. In *Inside Higher Ed*, Washington, DC, 2017.

365. Karukstis, K. K., Analysis of the Undergraduate Research Movement: Origins, Developments, and Current Challenges. *Scholarship and Practice of Undergraduate Research* **2019,** *3* (2), 46-55.

366. Theobald, K. J.; Hill, M. J.; Tran, E.; Agrawal, S.; Arroyo, E. N.; Behling, S.; Chambwe, N.; Cintron, D. L.; Cooper, J. D.; Dunster, G.; Grummer, J. A.; Hennessey, K.; Hsiao, J.; Iranon, N.; Jones, L.; Jordt, H.; Keller, M.; Lacey, M. E.; Littlefield, C. E.; Lowe, A.; Newman, S.; Okolo, V.; Olroyd, S.; Peecook, B. R.; Pickett, S. B.; Slager, D. L.; Caviedes-Solis, I. W.; Stanchak, K. E.; Sundaravardan, V.; Valebenito, C.; Williams, C. R.; Zinsli, K.; Freeman, S., Active learning narrows achievement gaps for underrepresented students in undergraduate science, technology, engineering, and math. *Proceedings of the National Academy of Sciences* **2020,** *PNAS Latest Articles*, 1-8.

367. Crowe, M.; Brakke, D., Assessing Undergraduate Research Experiences: An Annotative Bibliography. *Scholarship and Practice of Undergraduate Research* **2019,** *3* (2), 21-30.

368. Foertsch, J., Impacts of Undergraduate Research Programs Focused on Underrepresented Minorities: Twenty Years of Gradual Progress and Practices That Contributed to It. *Scholarship and Practice of Undergraduate Research* **2019,** *3* (2), 31-37.

369. Sorcinelli, M. D.; Yun, J., From Mentor to Mentoring Networks: Mentoring in the New Academy. *Change: The Magazine of Higher Learning* **2007,** *39* (6), 58-61.

370. Shields, G. C.; Hewitt, G. J.; North, L., Using Pre-College Research to Promote Student Success and Increase the Number of Science Majors. *CUR Quarterly* **2010,** *31* (1), 43-47.

371. Shields, G. C., Creating a Comprehensive Summer Undergraduate Research Program Despite Fiscal Challenges. *CUR Quarterly* **2010,** *30* (4), 18-21.

372. Oikawa, I.; Takamura, H., Correlation among Oxygen Vacancies, Protonic Defects, and the Acceptor Dopant in Sc-Doped BaZrO3 Studied by Sc-45 Nuclear Magnetic Resonance. *Chemistry of Materials* **2015,** *27* (19), 6660-6667.

373. Voter, A. F., Parallel replica method for dynamics of infrequent events. *Physical Review B* **1998,** *57* (22), 13985-13988.

374. Sorensen, M. R.; Voter, A. F., Temperature-accelerated dynamics for simulation of infrequent events. *J. Chem. Phys.* **2000,** *112* (21), 9599-9606.

375. Schultz, S. C.; Shields, G. C.; Steitz, T. A., Crystal structure of a CAP-DNA complex: the DNA is bent by 90 degrees. *Science* **1991,** *253* (5023), 1001-1007.

376. Sherer, E. C.; Yang, G.; Turner, G. M.; Shields, G. C.; Landry, D. W., Comparison of experimental and theoretical structures of a transition state analogue used for the induction of anti-cocaine catalytic antibodies. *J. Phys. Chem. A* **1997,** *101* (45), 8526-8529.

377. Shields, G. C.; Laughton, C. A.; Orozco, M., Molecular dynamics simulations of the d(T center dot A center dot T) triple helix. *Journal of the American Chemical Society* **1997,** *119* (32), 7463-7469.

378. Shields, G. C.; Laughton, C. A.; Orozco, M., Molecular dynamics simulation of a PNA center dot DNA center dot PNA triple helix in aqueous solution. *Journal of the American Chemical Society* **1998,** *120* (24), 5895-5904.

379. Jurema, M. W.; Shields, G. C., Ability of the PM3 quantum‐mechanical method to model *inter*molecular hydrogen bonding between neutral molecules. *Journal of Computational Chemistry* **1993,** *14* (1), 89-104.

380. Jurema, M. W.; Kirschner, K. N.; Shields, G. C., Modeling of magic water clusters (H2O)20 and (H2O)21H+ with the PM3 quantum‐mechanical method. *Journal of Computational Chemistry* **1993,** *14* (11), 1326-1332.

381. Kirschner, K. N.; Shields, G. C., Quantum-Mechanical Investigation of Large Water Clusters. *International Journal of Quantum Chemistry* **1994,** *52* (S28), 349-360.

382. Lu, J. H.; Li, H. T.; Liu, M. C.; Zhang, J. P.; Li, M.; An, X. M.; Chang, W. R., Crystal structure of human sulfotransferase SULT1A3 in complex with dopamine and 3 '-phosphoadenosine 5 '-phosphate. *Biochemical and Biophysical Research Communications* **2005,** *335* (2), 417-423.

383. Rote, J. C.; Malkowski, S. N.; Cochrane, C. S.; Bailey, G. E.; Brown, N. S.; Cafiero, M.; Peterson, L. W., Catechol reactivity: Synthesis of dopamine derivatives substituted at the 6-position. *Synthetic Communications* **2017,** *47* (5), 435-441.

384. Roldan, R. J.; Pajarillo, A. O.; Greenberg, J. D.; Karlinsey, J. E.; Cafiero, M.; Frawley, E. R.; Peterson, L. W., Propargylglycine-based antimicrobial compounds are targets of TolC-dependent efflux systems in Escherichia coli. *Bioorganic & Medicinal Chemistry Letters* **2020,** *30* (2), 126875.

385. Prasad, S.; Walker, N.; Henry, M.; Donald, K. J., Hop-Skip-Jump: Monovalent Metals on the Surface of the Phenalenyl Radical. *Organometallics* **2020,** *39* (1), 34-42.

386. Báez-Grez, R.; Inostroza, D.; García, V.; Vásquez-Espinal, A.; Donald, K. J.; Tiznado, W., Aromatic ouroboroi: heterocycles involving a σ-donor–acceptor bond and 4n + 2 π-electrons. *Phys. Chem. Chem. Phys.* **2020**.

387. Molinero, V.; Moore, E. B., Water Modeled As an Intermediate Element between Carbon and Silicon. *J. Phys. Chem. B* **2009,** *113* (13), 4008-4016.

388. DeMille, R. C.; Molinero, V., Coarse-grained ions without charges: Reproducing the solvation structure of NaCl in water using short-ranged potentials. *J. Chem. Phys.* **2009,** *131* (3).

389. Jacobson, L. C.; Hujo, W.; Molinero, V., Nucleation Pathways of Clathrate Hydrates: Effect of Guest Size and Solubility. *J. Phys. Chem. B* **2010,** *114* (43), 13796-13807.

390. Nagel, Z. D.; Klinman, J. P., Update 1 of: Tunneling and Dynamics in Enzymatic Hydride Transfer. *Chemical Reviews* **2010,** *110* (12), PR41-PR67.

391. Vina-Gonzalez, J.; Jimenez-Lalana, D.; Sancho, F.; Serrano, A.; Martinez, A. T.; Guallar, V.; Alcalde, M., Structure-Guided Evolution of Aryl Alcohol Oxidase from Pleurotus eryngii for the Selective Oxidation of Secondary Benzyl Alcohols. *Advanced Synthesis & Catalysis* **2019,** *361* (11), 2514-2525.

392. Eigner, A. A.; Rohde, J. A.; Knutson, C. C.; Phillips, J. A., IR Spectrum of CH3CN-BF3 in Solid Neon: Matrix Effects on the Structure of a Lewis Acid-Base Complex. *The Journal of Physical Chemistry B* **2007,** *111* (6), 1402-1407.

393. Phillips, J. A.; Cramer, C. J., B-N Distance Potential of CH3CN-BF3 Revisited: Resolving the Experiment-Theory Structure Discrepancy and Modeling the Effects of Low-Dielectric Environments. *The Journal of Physical Chemistry B* **2007,** *111* (6), 1408-1415.

394. Leopold, K. R.; Canagaratna, M.; Phillips, J. A., Partially bonded molecules from the solid state to the stratosphere. *Accounts of Chemical Research* **1997,** *30* (2), 57-64.

395. Phillips, J. A.; Halfen, J. A.; Wrass, J. P.; Knutson, C. C.; Cramer, C. J., Large gas-solid structural differences in complexes of haloacetonitriles with boron trifluoride. *Inorganic Chemistry* **2006,** *45* (2), 722-731.

396. Mike, J. F.; Nalwa, K.; Makowski, A. J.; Putnam, D.; Tomlinson, A. L.; Chaudhary, S.; Jeffries-El, M., Synthesis, characterization and photovoltaic properties of poly(thiophenevinylene-alt-benzobisoxazole)s. *Phys. Chem. Chem. Phys.* **2011,** *13* (4), 1338-1344.

397. Tlach, B. C.; Tomlinson, A. L.; Bhuwalka, A.; Jeffries-El, M., Tuning the Optical and Electronic Properties of 4,8-Disubstituted Benzobisoxazoles via Alkyne Substitution. *J. Org. Chem.* **2011,** *76* (21), 8670-8681.

398. Boutilier, K.; Ross, M.; Podtelejnikov, A. V.; Orsi, C.; Taylor, R.; Taylor, P.; Figeys, D., Comparison of different search engines using validated MS/MS test datasets. *Analytica Chimica Acta* **2005,** *534* (1), 11-20.

399. Miller, S. A.; Riederer, D. E.; Cooks, R. G.; Cho, W. R.; Lee, H. W.; Kang, H., Energy disposal and target effects in hyperthermal collisions of ferrocene molecular ions at surfaces. *Journal of Physical Chemistry* **1994,** *98* (1), 245-251.

400. McCormack, A. L.; Somogyi, A.; Dongre, A. R.; Wysocki, V. H., Fragmentation of protonated peptdes: surface-induced dissociation in conjunction with a quantum mechanical approach *Analytical Chemistry* **1993,** *65* (20), 2859-2872.

401. Laskin, J.; Denisov, E.; Futrell, J., A comparative study of collision-induced and surface-induced dissociation. 1. Fragmentation of protonated dialanine. *Journal of the American Chemical Society* **2000,** *122* (40), 9703-9714.

402. Wang, P.; Hadjar, O.; Gassman, P. L.; Laskin, J., Reactive landing of peptide ions on self-assembled monolayer surfaces: an alternative approach for covalent immobilization of peptides on surfaces. *Phys. Chem. Chem. Phys.* **2008,** *10* (11), 1512-1522.

403. Laskin, J.; Denisov, E.; Futrell, J., Comparative study of collision-induced and surface-induced dissociation. 2. Fragmentation of small alanine-containing peptides in FT-ICR MS. *J. Phys. Chem. B* **2001,** *105* (9), 1895-1900.

404. Douglas, D. J., Applications of collision dynamics in quadrupole mass spectrometry. *Journal of the American Society for Mass Spectrometry* **1998,** *9* (2), 101-113.

405. Dongre, A. R.; Jones, J. L.; Somogyi, A.; Wysocki, V. H., Influence of peptide composition, gas-phase basicity, and chemical modification on fragmentation efficiency: Evidence for the mobile proton model. *Journal of the American Chemical Society* **1996,** *118* (35), 8365-8374.

406. Paizs, B.; Suhai, S., Fragmentation pathways of protonated peptides. *Mass Spectrometry Reviews* **2005,** *24* (4), 508-548.

407. Morrison, L.; Somogyi, A.; Wysocki, V. H., The influence glutamic acid in protonated b(3) -> b(2) formation from VGEIG and related analogs. *International Journal of Mass Spectrometry* **2012,** *325*, 139-149.

408. Ijaz, W.; Gregg, Z.; Barnes, G. L., Complex Formation during SID and Its Effect on Proton Mobility. *Journal of Physical Chemistry Letters* **2013,** *4* (22), 3935-3939.

409. Gregg, Z.; Ijaz, W.; Jannetti, S.; Barnes, G. L., The Role of Proton Transfer in Surface-Induced Dissociation. *Journal of Physical Chemistry C* **2014,** *118* (38), 22149-22155.

410. Shaikh, K.; Blackwood, J.; Barnes, G. L., The effect of protonation site and conformation on surface-induced dissociation in a small, lysine containing peptide. *Chemical Physics Letters* **2015,** *637*, 83-87.

411. Geragotelis, A.; Barnes, G. L., Surface Deposition Resulting from Collisions between Diglycine and Chemically Modified Alkylthiolate Self-Assembled Monolayer Surfaces. *Journal of Physical Chemistry C* **2013,** *117* (25), 13087-13093.

412. Levi, L.; Wang, Z.; Doud, M. K.; Hazen, S. L.; Noy, N., Saturated fatty acids regulate retinoic acid signalling and suppress tumorigenesis by targeting fatty acid-binding protein 5. *Nature Communications* **2015,** *6*.

413. Kosenkov, Y. K.; Kosenkov, D., Quantum dynamics of vibration-assisted excitation energy transfer in phycobiliprotein light-harvesting complex. *The Journal of Chemical Physics* **2019,** *151* (14), 144101.

414. Ghosh, D.; Kosenkov, D.; Vanovschi, V.; Williams, C. F.; Herbert, J. M.; Gordon, M. S.; Schmidt, M. W.; Slipchenko, L. V.; Krylov, A. I., Noncovalent Interactions in Extended Systems Described by the Effective Fragment Potential Method: Theory and Application to Nucleobase Oligomers. *J. Phys. Chem. A* **2010,** *114* (48), 12739-12754.

415. James, W. H., III; Buchanan, E. G.; Mueller, C. W.; Dean, J. C.; Kosenkov, D.; Slipchenko, L. V.; Guo, L.; Reidenbach, A. G.; Gellman, S. H.; Zwier, T. S., Evolution of Amide Stacking in Larger gamma-Peptides: Triamide H-Bonded Cycles. *J. Phys. Chem. A* **2011,** *115* (47), 13783-13798.

416. Prato, G.; Silvent, S.; Saka, S.; Lamberto, M.; Kosenkov, D., Thermodynamics of Binding of Di- and Tetrasubstituted Naphthalene Diimide Ligands to DNA G-Quadruplex. *J. Phys. Chem. B* **2015,** *119* (8), 3335-3347.

417. Ghosh, D.; Kosenkov, D.; Vanovschi, V.; Flick, J.; Kaliman, I.; Shao, Y.; Gilbert, A. T. B.; Krylov, A. I.; Slipchenko, L. V., Effective fragment potential method in Q-CHEM: A guide for users and developers. *Journal of Computational Chemistry* **2013,** *34* (12), 1060-1070.

418. Flick, J. C.; Kosenkov, D.; Hohenstein, E. G.; Sherrill, C. D.; Slipchenko, L. V., Accurate Prediction of Noncovalent Interaction Energies with the Effective Fragment Potential Method: Comparison of Energy Components to Symmetry-Adapted Perturbation Theory for the S22 Test Set. *J. Chem. Theory Comput.* **2012,** *8* (8), 2835-2843.

419. Kosenkov, D.; Slipchenko, L. V., Solvent Effects on the Electronic Transitions of p-Nitroaniline: A QM/EFP Study. *J. Phys. Chem. A* **2011,** *115* (4), 392-401.

420. Seinfeld, J. H.; Pandis, S. N., *Atmospheric Chemistry and Physics: From Air Pollution to Climate Change*. 2nd ed.; John Wiley & Sons, Inc.: New York, 2006; p 1-1203.

421. Prather, K. A.; Hatch, C. D.; Grassian, V. H., Analysis of Atmospheric Aerosols. *Annual Review of Analytical Chemistry* **2008,** *1*, 485-514.

422. Finlayson-Pitts, B. J., Reactions at surfaces in the atmosphere: integration of experiments and theory as necessary (but not necessarily sufficient) for predicting the physical chemistry of aerosols. *Phys. Chem. Chem. Phys.* **2009,** *11* (36), 7760-7779.

423. Chen, H.; Navea, J. G.; Young, M. A.; Grassian, V. H., Heterogeneous Photochemistry of Trace Atmospheric Gases with Components of Mineral Dust Aerosol. *J. Phys. Chem. A* **2011,** *115* (4), 490-499.

424. Usher, C. R.; Michel, A. E.; Grassian, V. H., Reactions on mineral dust. *Chemical Reviews* **2003,** *103* (12), 4883-4939.

425. Linke, C.; Moehler, O.; Veres, A.; Mohacsi, A.; Bozoki, Z.; Szabo, G.; Schnaiter, M., Optical properties and mineralogical composition of different Saharan mineral dust samples: a laboratory study. *Atmospheric Chemistry and Physics* **2006,** *6*, 3315-3323.

426. Hanisch, F.; Crowley, J. N., Ozone decomposition on Saharan dust: an experimental investigation. *Atmospheric Chemistry and Physics* **2003,** *3*, 119-130.

427. Lesko, D. M. B.; Coddens, E. M.; Swomley, H. D.; Welch, R. M.; Borgatta, J.; Navea, J. G., Photochemistry of nitrate chemisorbed on various metal oxide surfaces. *Phys. Chem. Chem. Phys.* **2015,** *17* (32), 20775-20785.

428. Baltrusaitis, J.; Schuttlefield, J.; Jensen, J. H.; Grassian, V. H., FTIR spectroscopy combined with quantum chemical calculations to investigate adsorbed nitrate on aluminium oxide surfaces in the presence and absence of co-adsorbed water. *Phys. Chem. Chem. Phys.* **2007,** *9* (36), 4970-4980.

429. Galhotra, P.; Navea, J. G.; Larsen, S. C.; Grassian, V. H., Carbon dioxide ((CO2)-O-16 and (CO2)-O-18) adsorption in zeolite Y materials: effect of cation, adsorbed water and particle size. *Energy & Environmental Science* **2009,** *2* (4), 401-409.

430. Irikura, K. K.; Johnson, R. D.; Kacker, R. N., Uncertainties in Scaling Factors for ab Initio Vibrational Frequencies. *The Journal of Physical Chemistry A* **2005,** *109* (37), 8430-8437.

431. Wenzel, D. M.; Stoll, K. E.; Klevit, R. E., E2s: structurally economical and functionally replete. *Biochemical Journal* **2011,** *433*, 31-42.

432. Bedford, L.; Lowe, J.; Dick, L. R.; Mayer, R. J.; Brownell, J. E., Ubiquitin-like protein conjugation and the ubiquitin-proteasome system as drug targets. *Nature Reviews Drug Discovery* **2011,** *10* (1), 29-46.

433. Wu, P. Y.; Hanlon, M.; Eddins, M.; Tsui, C.; Rogers, R. S.; Jensen, J. P.; Matunis, M. J.; Weissman, A. M.; Wolberger, C. P.; Pickart, C. M., A conserved catalytic residue in the ubiquitin-conjugating enzyme family. *Embo Journal* **2003,** *22* (19), 5241-5250.

434. Tanner, K. G.; Trievel, R. C.; Kuo, M. H.; Howard, R. M.; Berger, S. L.; Allis, C. D.; Marmorstein, R.; Denu, J. M., Catalytic mechanism and function of invariant glutamic acid 173 from the histone acetyltransferase GCN5 transcriptional coactivator. *Journal of Biological Chemistry* **1999,** *274* (26), 18157-18160.

435. Berndsen, C. E.; Wiener, R.; Yu, I. W.; Ringel, A. E.; Wolberger, C., A conserved asparagine has a structural role in ubiquitin-conjugating enzymes. *Nature Chemical Biology* **2013,** *9* (3), 154-156.

436. Chen, H.; Ezell, M. J.; Arquero, K. D.; Varner, M. E.; Dawson, M. L.; Gerber, R. B.; Finlayson-Pitts, B. J., New particle formation and growth from methanesulfonic acid, trimethylamine and water. *Phys. Chem. Chem. Phys.* **2015,** *17* (20), 13699-13709.

437. Gerber, R. B.; Varner, M. E.; Hammerich, A. D.; Riikonen, S.; Murdachaew, G.; Shemesh, D.; Finlayson-Pitts, B. J., Computational Studies of Atmospherically-Relevant Chemical Reactions in Water Clusters and on Liquid Water and Ice Surfaces. *Accounts of Chemical Research* **2015,** *48* (2), 399-406.

438. Tschumper, G. S.; Ellington, T. L.; Johnson, S. N., Dissociation in Binary Acid/Base Clusters: An Examination of Inconsistencies Introduced Into the Many-Body Expansion by Naive Fragmentation Schemes. In *Annual Reports in Computational Chemistry, Vol 13*, Dixon, D. A., Ed. 2017; Vol. 13, pp 93-115.

439. Johnson, S. N.; Hutchison, C. R.; Williams, C. M.; Hus, H. L.; Tschumper, G. S.; Hammer, N. I., Intermolecular Interactions and Vibrational Perturbations within Mixtures of 1-Ethyl-3-methylimidazolium Thiocyanate and Water. *Journal of Physical Chemistry C* **2018,** *122* (48), 27673-27680.

440. Johnson, S. N.; Tschumper, G. S., Hydrogen bonding in the mixed HF/HCl dimer: Is it better to give or receive? *Journal of Computational Chemistry* **2018,** *39* (14), 839-843.

441. Johnson, S. N.; Ellington, T. L.; Ngo, D. T.; Nevarez, J. L.; Sparks, N.; Rheingold, A. L.; Watkins, D. L.; Tschumper, G. S., Probing non-covalent interactions driving molecular assembly in organo-electronic building blocks. *Crystengcomm* **2019,** *21* (20), 3151-3157.

442. Biais, N.; Higashi, D. L.; Brujić, J.; So, M.; Sheetz, M. P., Force-dependent polymorphism in type IV pili reveals hidden epitopes. *Proceedings of the National Academy of Sciences* **2010,** *107* (25), 11358-11363.

443. Baker, J. L.; Biais, N.; Tama, F., Steered Molecular Dynamics Simulations of a Type IV Pilus Probe Initial Stages of a Force-Induced Conformational Transition. *Plos Computational Biology* **2013,** *9* (4).

444. Baker, J. L.; Furbish, J.; Lindberg, G. E., Influence of the ionic liquid C(4)mpy Tf2N on the structure of the miniprotein Trp-cage. *Journal of Molecular Graphics & Modelling* **2015,** *62*, 202-212.

445. Kojima, A.; Teshima, K.; Shirai, Y.; Miyasaka, T., Organometal Halide Perovskites as Visible-Light Sensitizers for Photovoltaic Cells. *Journal of the American Chemical Society* **2009,** *131* (17), 6050-+.

446. Wrighton, M. S.; Ellis, A. B.; Wolczanski, P. T.; Morse, D. L.; Abrahamson, H. B.; Ginley, D. S., Strontium-titanate photoelectrodes: efficient photoassisted electrolysis of water at zero applied potential. *Journal of the American Chemical Society* **1976,** *98* (10), 2774-2779.

447. Mavroides, J. G.; Kafalas, J. A.; Kolesar, D. F., Photoelectrolysis of water in cells with SrTiO3 anodes. *Applied Physics Letters* **1976,** *28* (5), 241-243.

448. Daly, C. A.; Berquist, E. J.; Brinzer, T.; Garrett-Roe, S.; Lambrecht, D. S.; Corcelli, S. A., Modeling Carbon Dioxide Vibrational Frequencies in Ionic Liquids: II. Spectroscopic Map. *J. Phys. Chem. B* **2016,** *120* (49), 12633-12642.

449. Berquist, E. J.; Daly, C. A.; Brinzer, T.; Bullard, K. K.; Campbell, Z. M.; Corcelli, S. A.; Garrett-Roe, S.; Lambrecht, D. S., Modeling Carbon Dioxide Vibrational Frequencies in Ionic Liquids: I. Ab Initio Calculations. *J. Phys. Chem. B* **2017,** *121* (1), 208-220.

450. Daly, C. A.; Streacker, L. M.; Sun, Y. C.; Pattenaude, S. R.; Hassanali, A. A.; Petersen, P. B.; Corcelli, S. A.; Ben-Arnotz, D., Decomposition of the Experimental Raman and Infrared Spectra of Acidic Water into Proton, Special Pair, and Counterion Contributions. *Journal of Physical Chemistry Letters* **2017,** *8* (21), 5246-5252.

451. Brinzer, T.; Daly, C. A.; Allison, C.; Garrett-Roe, S.; Corcelli, S. A., Modeling Carbon Dioxide Vibrational Frequencies in Ionic Liquids: III. Dynamics and Spectroscopy. *J. Phys. Chem. B* **2018,** *122* (38), 8931-8942.

452. Daly, C. A.; Brinzer, T.; Allison, C.; Garrett-Roe, S.; Corcelli, S. A., Enthalpic Driving Force for the Selective Absorption of CO2 by an Ionic Liquid. *Journal of Physical Chemistry Letters* **2018,** *9* (6), 1393-1397.

453. Daly, C. A.; Allison, C.; Corcelli, S. A., Modeling Carbon Dioxide Vibrational Frequencies in Ionic Liquids: IV. Temperature Dependence. *J. Phys. Chem. B* **2019,** *123* (17), 3797-3803.

454. Drexler, C. I.; Miller, T. C.; Rogers, B. A.; Li, Y. G. C.; Daly, C. A.; Yang, T. L.; Corcelli, S. A.; Cremer, P. S., Counter Cations Affect Transport in Aqueous Hydroxide Solutions with Ion Specificity. *Journal of the American Chemical Society* **2019,** *141* (17), 6930-6936.

455. Derricotte, W. D., Symmetry-Adapted Perturbation Theory Decomposition of the Reaction Force: Insights into Substituent Effects Involved in Hemiacetal Formation Mechanisms. *The Journal of Physical Chemistry A* **2019,** *123* (36), 7881-7891.

456. Zhang, N.; Han, C.; Xu, Y.-J.; Foley Iv, J. J.; Zhang, D.; Codrington, J.; Gray, S. K.; Sun, Y., Near-field dielectric scattering promotes optical absorption by platinum nanoparticles. *Nature Photonics* **2016,** *10* (7), 473-482.

457. Codrington, J.; Eldabagh, N.; Fernando, K.; Foley, J. J., Unique Hot Carrier Distributions from Scattering-Mediated Absorption. *Acs Photonics* **2017,** *4* (3), 552-559.

458. Eldabagh, N.; Micek, M.; DePrince, A. E.; Foley, J. J., Resonance Energy Transfer Mediated by Metal-Dielectric Composite Nanostructures. *Journal of Physical Chemistry C* **2018,** *122* (32), 18256-18265.

459. Varner, J. F.; Eldabagh, N.; Volta, D.; Eldabagh, N.; Foley IV, J. J., WPTherml: A Python Package for the Design of Materials for Harnessing Heat. *Journal of Open Research Software* **2019,** *7* (1).

460. Varner, J. F.; Wert, D.; Matari, A.; Nofal, R.; Foley, J. J., Accelerating the discovery of multilayer nanostructures with analytic differentiation of the transfer matrix equations. *Phys. Rev. Research* **2020,** *2* (1).

461. He, K. D.; Allen, W. D., Conformers of Gaseous Serine. *J. Chem. Theory Comput.* **2016,** *12* (8), 3571-3582.

462. Xu, R. J.; Blasiak, B.; Cho, M.; Layfield, J. P.; Londergan, C. H., A Direct, Quantitative Connection between Molecular Dynamics Simulations and Vibrational Probe Line Shapes. *The Journal of Physical Chemistry Letters* **2018,** *9* (10), 2560-2567.

463. Perkyns, J. S.; Lynch, G. C.; Howard, J. J.; Pettitt, B. M., Protein solvation from theory and simulation: Exact treatment of Coulomb interactions in three-dimensional theories. *The Journal of Chemical Physics* **2010,** *132* (6), 064106.

464. Luchko, T.; Gusarov, S.; Roe, D. R.; Simmerling, C.; Case, D. A.; Tuszynski, J.; Kovalenko, A., Three-Dimensional Molecular Theory of Solvation Coupled with Molecular Dynamics in Amber. *J. Chem. Theory Comput.* **2010,** *6* (3), 607-624.

465. Johnson, J.; Case, D. A.; Yamazaki, T.; Gusarov, S.; Kovalenko, A.; Luchko, T., Small molecule hydration energy and entropy from 3D-RISM. *Journal of Physics-Condensed Matter* **2016,** *28* (34).

466. Luchko, T.; Blinov, N.; Limon, G. C.; Joyce, K. P.; Kovalenko, A., SAMPL5: 3D-RISM partition coefficient calculations with partial molar volume corrections and solute conformational sampling. *Journal of Computer-Aided Molecular Design* **2016,** *30* (11), 1115-1127.

467. Genheden, S.; Luchko, T.; Gusarov, S.; Kovalenko, A.; Ryde, U., An MM/3D-RISM Approach for Ligand Binding Affinities. *J. Phys. Chem. B* **2010,** *114* (25), 8505-8516.

468. Giambasu, G. M.; Luchko, T.; Herschlag, D.; York, D. M.; Case, D. A., Ion Counting from Explicit-Solvent Simulations and 3D-RISM. *Biophysical Journal* **2014,** *106* (4), 883-894.

469. Giambasu, G. M.; Gebala, M. K.; Panteva, M. T.; Luchko, T.; Case, D. A.; York, D. M., Competitive interaction of monovalent cations with DNA from 3D-RISM. *Nucleic Acids Research* **2015,** *43* (17), 8405-8415.

470. Nguyen, C.; Yamazaki, T.; Kovalenko, A.; Case, D. A.; Gilson, M. K.; Kurtzman, T.; Luchko, T., A molecular reconstruction approach to site-based 3D-RISM and comparison to GIST hydration thermodynamic maps in an enzyme active site. *Plos One* **2019,** *14* (7).

471. Tsednee, T.; Luchko, T., Closure for the Ornstein-Zernike equation with pressure and free energy consistency. *Physical Review E* **2019,** *99* (3).

472. Miller, S. L., Clathrate Hydrates of Air in Antarctic Ice. *Science* **1969,** *165* (3892), 489-&.

473. Archer, D.; Buffett, B.; Brovkin, V., Ocean methane hydrates as a slow tipping point in the global carbon cycle. *Proc. Natl. Acad. Sci. U. S. A.* **2009,** *106* (49), 20596-20601.

474. Kvenvolden, K. A., METHANE HYDRATES AND GLOBAL CLIMATE. *Global Biogeochemical Cycles* **1988,** *2* (3), 221-229.

475. Sloan, E. D., Fundamental principles and applications of natural gas hydrates. *Nature* **2003,** *426* (6964), 353-359.

476. Chatti, I.; Delahaye, A.; Fournaison, L.; Petitet, J. P., Benefits and drawbacks of clathrate hydrates: a review of their areas of interest. *Energy Conversion and Management* **2005,** *46* (9-10), 1333-1343.

477. Ghosh, J.; Methikkalam, R. R. J.; Bhuin, R. G.; Ragupathy, G.; Choudhary, N.; Kumar, R.; Pradeep, T., Clathrate hydrates in interstellar environment. *Proc. Natl. Acad. Sci. U. S. A.* **2019,** *116* (5), 1526-1531.

478. Desmedt, A.; Martin-Gondre, L.; Nguyen, T. T.; Petuya, C.; Barandiaran, L.; Babot, O.; Toupance, T.; Grim, R. G.; Sum, A. K., Modifying the Flexibility of Water Cages by Co-Including Acidic Species within Clathrate Hydrate. *Journal of Physical Chemistry C* **2015,** *119* (16), 8904-8911.

479. Ikeda, T.; Mae, S.; Uchida, T., Effect of guest-host interaction on Raman spectrum of a CO2 clathrate hydrate single crystal. *J. Chem. Phys.* **1998,** *108* (4), 1352-1359.

480. Jia, J. H.; Liang, Y. F.; Tsuji, T.; Murata, S.; Matsuoka, T., Elasticity and Stability of Clathrate Hydrate: Role of Guest Molecule Motions. *Scientific Reports* **2017,** *7*.

481. Nada, H., Growth mechanism of a gas clathrate hydrate from a dilute aqueous gas solution: A molecular dynamics simulation of a three-phase system. *J. Phys. Chem. B* **2006,** *110* (33), 16526-16534.

482. Cao, X. X.; Su, Y.; Zhao, J. J., Stability and Vibrations of Guest Molecules in the Type II Clathrate Hydrate: A First-Principles Study of Solid Phase. *J. Phys. Chem. A* **2015,** *119* (27), 7063-7069.

483. Srivastava, H. K.; Sastry, G. N., Viability of Clathrate Hydrates as CO2 Capturing Agents: A Theoretical Study. *J. Phys. Chem. A* **2011,** *115* (26), 7633-7637.

484. Qu, C.; Bowman, J. M., Ab Initio, Embedded Local-Monomer Calculations of Methane Vibrational Energies in Clathrate Hydrates. *Journal of Physical Chemistry C* **2016,** *120* (6), 3167-3175.

485. Lu, Q. N.; He, X.; Hu, W. X.; Chen, X. J.; Liu, J. F., Stability, Vibrations, and Diffusion of Hydrogen Gas in Clathrate Hydrates: Insights from Ab Initio Calculations on Condensed-Phase Crystalline Structures. *Journal of Physical Chemistry C* **2019,** *123* (19), 12052-12061.

486. Tinsley, M. R.; Nkomo, S.; Showalter, K., Chimera and phase-cluster states in populations of coupled chemical oscillators. *Nature Physics* **2012,** *8* (9), 662-665.

487. Nkomo, S.; Tinsley, M. R.; Showalter, K., Chimera States in Populations of Nonlocally Coupled Chemical Oscillators. *Physical Review Letters* **2013,** *110* (24).

488. Nkomo, S.; Tinsley, M. R.; Showalter, K., Chimera and chimera-like states in populations of nonlocally coupled homogeneous and heterogeneous chemical oscillators. *Chaos* **2016,** *26* (9).

489. Sanganyado, E.; Nkomo, S., Incorporating Sustainability into Engineering and Chemical Education Using E-Learning. *Education Sciences* **2018,** *8* (2).

490. Gzyl, A. S.; Oliynyk, A. O.; Adutwum, L. A.; Mar, A., Solving the Coloring Problem in Half-Heusler Structures: Machine Learning Predictions and Experimental Validation. *Inorganic Chemistry* **2019,** *58* (14), 9280-9289.

491. Matlinska, M. A.; Ha, M.; Hughton, B.; Oliynyk, A. O.; Iyer, A. K.; Bernard, G. M.; Lambkin, G.; Lawrence, M. C.; Katz, M. J.; Mar, A.; Michaelis, V. K., Alkaline Earth Metal-Organic Frameworks with Tailorable Ion Release: A Path for Supporting Biomineralization. *Acs Applied Materials & Interfaces* **2019,** *11* (36), 32739-32745.

492. Oliynyk, A. O.; Buriak, J. M., Virtual Issue on Machine-Learning Discoveries in Materials Science. *Chemistry of Materials* **2019,** *31* (20), 8243-8247.

493. Tehrani, A. M.; Oliynyk, A. O.; Rizvi, Z.; Lotfi, S.; Parry, M.; Sparks, T. D.; Brgoch, J., Atomic Substitution to Balance Hardness, Ductility, and Sustainability in Molybdenum Tungsten Borocarbide. *Chemistry of Materials* **2019,** *31* (18), 7696-7703.

494. Viswanathan, G.; Oliynyk, A. O.; Antono, E.; Ling, J.; Meredig, B.; Brgoch, J., Single-Crystal Automated Refinement (SCAR): A Data-Driven Method for Determining Inorganic Structures. *Inorganic Chemistry* **2019,** *58* (14), 9004-9015.

495. Zhou, Y. Q.; Iyer, A. K.; Oliynyk, A. O.; Heyberger, M.; Lin, Y. X.; Qiu, Y.; Mar, A., Quaternary rare-earth sulfides RE3M0.5M ' S-7 (M = Zn, Cd; M ' = Si, Ge). *Journal of Solid State Chemistry* **2019,** *278*.

496. Scott, C. E.; Kendall, D. A., Assessing Allosteric Modulation of CB1 at the Receptor and Cellular Levels. In *Cannabinoids and Their Receptors*, Reggio, P. H., Ed. 2017; Vol. 593, pp 317-342.

497. Ogawa, L. M.; Burford, N. T.; Liao, Y. H.; Scott, C. E.; Hine, A. M.; Dowling, C.; Chin, J.; Power, M.; Hunnicutt, E. J.; Emerick, V. L.; Banks, M.; Zhang, L. T.; Gerritz, S. W.; Alt, A.; Kendall, D. A., Discovery of Selective Cannabinoid CB2 Receptor Agonists by High-Throughput Screening. *Slas Discovery* **2018,** *23* (4), 375-383.

498. Stewart, B. D.; Scott, C. E.; McCoy, T. P.; Yin, G.; Despa, F.; Despa, S.; Kekenes-Huskey, P. M., Computational modeling of amylin-induced calcium dysregulation in rat ventricular cardiomyocytes. *Cell Calcium* **2018,** *71*, 65-74.

499. Kekenes-Huskey, P. M.; Scott, C. E.; Atalay, S., Quantifying the Influence of the Crowded Cytoplasm on Small Molecule Diffusion. *J. Phys. Chem. B* **2016,** *120* (33), 8696-8706.

500. Kucharski, A. N.; Scott, C. E.; Davis, J. P.; Kekenes-Huskey, P. M., Understanding Ion Binding Affinity and Selectivity in beta-Parvalbumin Using Molecular Dynamics and Mean Spherical Approximation Theory. *J. Phys. Chem. B* **2016,** *120* (33), 8617-8630.

501. Scott, C. E.; Ahn, K. H.; Graf, S. T.; Goddard, W. A.; Kendall, D. A.; Abrol, R., Computational Prediction and Biochemical Analyses of New Inverse Agonists for the CB1 Receptor. *Journal of Chemical Information and Modeling* **2016,** *56* (1), 201-212.

502. Ahn, K. H.; Scott, C. E.; Abrol, R.; Goddard, W. A.; Kendall, D. A., Computationally-predicted CB1 cannabinoid receptor mutants show distinct patterns of salt-bridges that correlate with their level of constitutive activity reflected in G protein coupling levels, thermal stability, and ligand binding. *Proteins-Structure Function and Bioinformatics* **2013,** *81* (8), 1304-1317.

503. Scott, C. E.; Abrol, R.; Ahn, K. H.; Kendall, D. A.; Goddard, W. A., Molecular basis for dramatic changes in cannabinoid CB1 G protein-coupled receptor activation upon single and double point mutations. *Protein Science* **2013,** *22* (1), 101-113.

504. Bray, J. K.; Abrol, R.; Goddard, W. A.; Trzaskowski, B.; Scott, C. E., SuperBiHelix method for predicting the pleiotropic ensemble of G-protein-coupled receptor conformations. *Proc. Natl. Acad. Sci. U. S. A.* **2014,** *111* (1), E72-E78.

505. Hauser, A. S.; Chavali, S.; Masuho, I.; Jahn, L. J.; Martemyanov, K. A.; Gloriam, D. E.; Babu, M. M., Pharmacogenomics of GPCR Drug Targets. *Cell* **2018,** *172* (1-2), 41-+.

506. Sigurdson, C. J.; Bartz, J. C.; Glatzel, M., Cellular and Molecular Mechanisms of Prion Disease. In *Annual Review of Pathology: Mechanisms of Disease, Vol 14*, Abbas, A. K.; Aster, J. C.; Feany, M. B., Eds. 2019; Vol. 14, pp 497-516.

507. Deleault, N. R.; Harris, B. T.; Rees, J. R.; Supattapone, S., Formation of native prions from minimal components in vitro. *Proc. Natl. Acad. Sci. U. S. A.* **2007,** *104* (23), 9741-9746.

508. Grabenauer, M.; Wu, C.; Soto, P.; Shea, J. E.; Bowers, M. T., Oligomers of the Prion Protein Fragment 106-126 Are Likely Assembled from beta-Hairpins in Solution, and Methionine Oxidation Inhibits Assembly without Altering the Peptide's Monomeric Conformation. *Journal of the American Chemical Society* **2010,** *132* (2), 532-539.

509. Soto, P.; Claflin, I. A.; Bursott, A. L.; Schwab-McCoy, A. D.; Bartz, J. C., Cellular prion protein gene polymorphisms linked to differential scrapie susceptibility correlate with distinct residue connectivity between secondary structure elements. *Journal of Biomolecular Structure and Dynamics* **2020**, 1-11.