NOMINATION SIGNATURE PAGE

2024 Virginia Outstanding Faculty Awards

Nominations must include this as the cover page of the nomination package PDF submission

Name of Applicant:	Daniel Crawford, PhD
Institution:	Virginia Tech
Category (choose only one): • Baccalaureate Institution • Masters/Comprehensive Institution • Research/Doctoral Institution • Two-Year Institution • Rising Star	Research/Doctoral Institution
Signature of President or Chief Academic Officer:	
Printed Name of President or Chief Academic Officer:	Cyril R. Clarke
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Mission Statement

Inspired by our land-grant identity and guided by our motto, *Ut Prosim* (That I May Serve), Virginia Tech is an inclusive community of knowledge, discovery, and creativity dedicated to improving the quality of life and the human condition within the Commonwealth of Virginia and throughout the world.

Summary of Accomplishments

Over his 23-year academic career, University Distinguished Professor T. Daniel Crawford has had a profound impact on research and education in the molecular sciences at Virginia Tech and on a global scale. He founded and nurtured a world-class research program in theoretical and computational chemistry that now includes five internationally recognized faculty members and their teams of graduate students and postdocs. His own research in the field of molecular quantum mechanics has resulted in more than 150 peer-reviewed publications and garnered numerous national and international awards. Prof. Crawford is regarded by both students and colleagues as one of the clearest communicators in his field in the world, and he has presented nearly 230 invited lectures at conferences and universities in 26 countries. He founded and currently directs the Molecular Sciences Software Institute (MolSSI), which is a nexus for collaboration, education, and research for the global computational chemistry community. He raised the bar for education in the molecular sciences both at the local level with his teaching of undergraduate and graduate students, and internationally through the MolSSI's ambitious instructional program that continues to reach thousands of students around the world each year. He has served the global molecular sciences community through numerous leadership roles, not only via his shepherding of the MolSSI, but also as an officer in and Fellow of the American Chemical Society and through more than a decade as an editor of the *Journal of Physical Chemistry*.

Teaching: Prof. Crawford's principal educational focus over his entire career has been the training of the next generation of computational molecular scientists, developing and teaching curricula spanning high-school, undergraduate, graduate, and postdoctoral levels of instruction and reaching tens of thousands of students worldwide. While his early efforts naturally emphasized quantum chemistry (his area of research), his teaching now spans the entire domain of molecular science, from electronic structure theory to bio-/macro-molecular simulation, to computational materials science. In all these demanding — and often intimidating — subjects. Prof. Crawford's overarching teaching philosophy contains four key components: (1) never "dumb down" the explanation of any subject, (2) communicate every concept as clearly and carefully as possible, (3) treat every student (and every student's question) with the utmost respect, and (4) always be empathetic and approachable. These evergreen principles have served as the foundation of his tremendous success as a teacher, as evident in his superb teaching evaluations and numerous teaching awards.

Prof. Crawford has long been an innovator in the education of the next generation of molecular scientists. Soon after he began his appointment in May of 2000 as an assistant professor at Virginia Tech, he introduced a series of "computational experiments" at all levels of the undergraduate chemistry laboratory curriculum. These educational components provided students with the opportunity to "play" with the quantum mechanics, thus making the learning process both more active and enjoyable. In addition, by coupling these computational experiments to lectures that teach the underlying physics, chemistry, and mathematics of the theory, students avoid the common "black box" phenomenon that leads them to believe anything the computer tells them. Thus, while these projects were intended to teach the power of modern computational chemistry to budding scientists and engineers, they were also designed to demonstrate the *limitations* of even state-of-the-art models.

Prof. Crawford's educational efforts have also extended well beyond the Virginia Tech campus. Starting in 2005, he developed a series of online, self-guided programming exercises with the goal of training his own graduate students in the fundamentals of the C and C++ languages using the context of basic electronic structure theory. Two years later, after numerous requests by collaborators and colleagues in the field, he made these exercises publicly available, and their usage soon grew to more than 100 computational chemistry groups worldwide, as

evidenced by more than 300 GitHub stars and more than 130 forks (both reliable proxies to estimate the impact of software). Prof. Crawford's skill as a communicator of challenging concepts is also evident in a series of video presentations that he prepared to supplement the educational resources of his lecture courses and summer schools, ranging from undergraduate physical chemistry to advanced topics in software development for the molecular sciences. One of these, a presentation on "Atomic Term Symbols," has garnered more than 79,000 views and more than 2,200 followers on YouTube, and the student comments (mostly from international viewers) on these videos are overwhelmingly and enthusiastically positive. Since 2019, he has served as the first and only American instructor for the prestigious European Summer School on Quantum Chemistry, which has been held biennially since 1989 (and for the last 18 years in Palermo, Sicily), and he has agreed to launch a North American version of the school beginning in 2025.

Discovery: Prof. Crawford's research has focused on the development and application of the most robust, reliable, and efficient quantum mechanical models of chemical compounds and reactions, particularly those of *chiral molecules.* Chirality is an inherent three-dimensional "handedness," a property found in all sugars, proteins, and enzymes, as well as most modern drugs. The two hands of a chiral compound can exhibit dramatically differing chemical behavior when reacting in a chiral environment, such as the human metabolism. A sinister example of such behavior is found in thalidomide, a drug prescribed to pregnant women in Europe in the 1950s as a sedative for morning sickness, but quickly removed from the market after it was found to cause serious birth defects. Later studies partially explained this horror, concluding that one hand of the chiral compound is the desired sedative while the other is a teratogen responsible for the damage to fetal tissue. Although organic chemists can routinely determine the purity of such compounds, the synthetic identification of each hand involves a process that can sometimes require *decades* to complete. However, the two hands of a chiral compound also exhibit differing responses to polarized light—responses that can be directly measured using a variety of both common and sophisticated spectroscopic methods. However, without an external reference, even these techniques cannot assign a given measurement to a particular hand of the compound. As a result, the experimental identification of the handedness of chiral drugs annually costs the global pharmaceutical industry hundreds of millions of dollars.

Prof. Crawford has dedicated most of his research over the last 20+ years to solving this fundamental problem of chemistry, specifically through developing advanced, first-principles quantum mechanical methods for *predicting* the optical properties of chiral molecules. Through dozens of synergistic collaborations with both experimentalists and theoreticians worldwide, his group's work has exposed the fundamental requirements of a physically correct quantum mechanical model for the interaction of electromagnetic radiation with chiral compounds, i.e., how to obtain "the right answer for the right reason." As a result, his group has performed arguably *the world's most sophisticated and robust computations of chiroptical spectra to date*.

Prof. Crawford's more than 150 peer-reviewed papers have garnered nearly 11,000 citations, and he has more than 20 papers with more than 100 citations each, with three above or approaching 1,000 citations each. Among Prof. Crawford's dozens of papers specifically on chiroptical spectroscopy, his foundational paper, "*Ab Initio* Calculation of Molecular Chiroptical Properties," [*Theor. Chem. Acc.,* 115, 227 (2006)] has had the highest impact. This work has provided the foundation for much of his own work in the area, as well as that of many other scientists, as evidenced by the more than 400 citations the work has earned. Another of Prof. Crawford's pivotal papers was published in his first year as an assistant professor in 2000: "An Introduction to Coupled Cluster Theory," [*Rev. Comp. Chem.*, 14, 33 (2000)]. The paper has been cited nearly 1,000 times and is used as a primary source by dozens of research groups around the world.

One of the major products of this work is the open-source quantum chemical program package PSI (psicode.org), of which Prof. Crawford has been a major developer for 30 years and through which he makes all of the computational tools he designs and builds freely available to the global community of computational scientists. The PSI code is used by the global quantum chemistry community for a broad spectrum of scientific problems, from conventional quantum chemistry to high-impact applications such as machine learning and quantum computing. Information about PSI is available at the main distribution website, the development site where the large programming team interacts, and the user/programmer forum which has 920 users and has received more than 1.65M pageviews since the team began collecting analytics in July 2015. The GitHub repository has nearly 850 stars and more than 400 forks, and the code has been downloaded more than 170,000 times in the last year alone. The four peer-reviewed papers on the PSI code have garnered nearly 3,000 citations, and the most recent paper (2020) has already been cited nearly 500 times.

The NSF has supported Prof. Crawford's research program continuously since 2001, and he has received nearly 30 generous grants from the NSF, the Dreyfus Foundation, the Research Corporation for Science Advancement, the Department of Energy, the Air Force Office of Scientific Research, and others for a total of approximately $41.8M in support. Prof. Crawford's impact on the field of quantum chemistry has been recognized by numerous international scientific societies. In 2010, he was selected as the winner of the Paul A.M. Dirac Medal of the World Association of Theoretical and Computational Chemists (WATOC) for the "Outstanding Computational Chemist under the Age of 40." He formally received this award at the WATOC Congress in Santiago de Compostela, Spain, in 2011, where he gave a plenary lecture to the conference's 1,300 participants. In 2022, Prof. Crawford was elected to membership in the International Academy of Quantum Molecular Science, the most prestigious and influential organization in his field. The IAQMS was established in 1967 in Menton, France, and includes only 124 elected members from around the world. Its current and past membership boasts 14 Nobel laureates, including Linus Pauling (chemistry, 1954; peace, 1962), Louis de Broglie (physics, 1929), Robert Mulliken (chemistry, 1966), and John Pople (chemistry, 1998).

Knowledge Integration: On a national and international level, Prof. Crawford has revolutionized training in the broader field of computational molecular science—quantum chemistry, bio- and macro-molecular simulation, and computational materials science – with the goal of helping the field solve ever larger and more complex problems. The molecular science community has made innumerable vital contributions to scientific discovery — from drug design to the development of new energy storage materials — such that computational chemistry is now regarded as a "full partner with experiment." Such scientific breakthroughs have been made possible by the evolution of hundreds of community software packages, including the PSI code described above, some with lifetimes reaching back to the earliest days of computing. The pivotal educational challenge, however, is how to equip newcomers to the field with the skills they need to contribute to such intricate and intimidating programs, many of which involve millions of lines of hand-written code in an amalgam of programming languages. Exacerbating this challenge is the inadequacy of chemistry and physics curricula (both undergraduate and graduate), which typically neglect instruction in programming and software design.

In 2016, Prof. Crawford launched the Molecular Sciences Software Institute (MolSSI), which is supported by the U.S. National Science Foundation through two five-year grants totaling $34.42M. He designed the MolSSI in collaboration with researchers at seven other elite U.S. universities to serve and enhance the software development efforts of the global community of computational molecular scientists by providing software infrastructure, by enabling the adoption of standards and best practices, *and by training the next generation of software engineers in computational chemistry*. To that end, Prof. Crawford established the MolSSI's Software

Fellowship Program – which has provided both financial support and mentorship to 115 graduate students and postdocs across the U.S. – and its Educational Initiative to provide summer schools, targeted workshops, undergraduate programs, and online curricula in order to shoulder the burden of training the field's future molecular scientists in modern software engineering. *To date the MolSSI's Educational Initiative has reached more than 2,500 students in face-to-face instruction (more than 500 in 2023 alone), and its on-line curricula and asynchronous delivery reach ca. 5,000 students each month worldwide.*

The MolSSI's Education Initiative and Fellowship Program have also been exceptionally successful in attracting members of underrepesented groups. For example, in 2020, the MolSSI's summer webinars (launched when the COVID-19 pandemic first struck) engaged 48% female participants and 22% underrepresented minorites. In collaboration with the MERCURY Consortium, for the last six years Prof. Crawford and the MolSSI team have organized a one-day undergraduate workshop on software development for molecular simulation at Furman University. Each workshop has been attended by ca. 30 students (55-60% female and 25-30% underrepresented minorities) and numerous faculty — all from primarily undergraduate institutions — and focused on the inner workings of molecular dynamics and quantum chemistry software packages. For the last five years, the MolSSI has collaborated with the Tapia Center for Excellence and Equity in Education to provide week-long coding workshops at Rice University specifically reaching underrepresented groups. The most recent workshop in 2023 included a student cohort that was 50% female, 40% Hispanic, and 20% African American.

Only by educating the next generation of molecular scientists in the best practices of modern software design and engineering will the field be prepared to tackle the next level of scientific Grand Challenges. Prof. Crawford's ultimate goal is to change fundamentally the software development enterprise — both education and culture — of the entire computational molecular sciences community.

Service: Prof. Crawford exemplifies Virginia Tech's motto, *Ut Prosim* (That I May Serve), by combining his passion for teaching with his expertise as a researcher to create programs in the service of others. For example, starting in 2013 (several years prior to founding the MolSSI), Prof. Crawford launched a series of "Software Summer Schools" targeting junior graduate students across the U.S. whose research required them to engage in sophisticated levels of software engineering and development. These intense, 10-day events covered a wide range of topics, including computing fundamentals and best practices, version-control repositories, build systems, debugging tools, high-performance computing architectures, parallel computing, and more, all oriented toward newcomers to electronic structure theory.

Prof. Crawford has a deep commitment to serving the Virginia Tech community, having served on (and often chaired) numerous committees in the Department of Chemistry, the College of Science, and the University, including as a member of the Virginia Tech President's Advisory Council. Prof. Crawford has demonstrated an equally impressive commitment to serving his professional community. In addition to his role as Director of the MolSSI (2016-present), he has served as Deputy Editor of the *Journal of Physical Chemistry A* (2021-present), Senior Editor of *Journal of Physical Chemistry* (2012-2020), and Secretary/Treasurer of the Physical Chemistry (PHYS) Division of the American Chemical Society (2012-2017). He has also organized 13 conferences, including six ACS symposia and three major international meetings (such as the 10th Molecular Quantum Mechanics conference at Virginia Tech in summer 2022), and he has served as a peer reviewer for dozens of journals, including *Science*, *Nature Chemistry*, and the *Journal of the American Chemical Society*.

Personal Statement

I was raised on a beef cattle farm in north Alabama, and, until I departed for college, I attended rural public schools with teachers who were knowledgeable, conscientious, and caring. My parents taught me the value of education, hard work, and respect for others. They reminded me on numerous occasions: "Everyone knows something that you don't, no matter where they're from, what they do for a living, or where (or even if) they went to school. Treat everyone you meet with respect, and maybe they'll teach you something new." I have tried to live my life by this important truth.

I discovered at an early age that the best way to learn is to teach, and this realization has profoundly influenced my entire academic career – indeed, much of my way of life. In my sixth-grade science class, the teacher assigned me the task of tutoring one of my peers, and over a two-month period, I worked closely with my fellow student to help him understand more deeply the basic scientific concepts we were learning in class. I soon found that my own comprehension of the subject expanded dramatically as I worked to organize my thoughts so I could convey them clearly to my friend. A few years later in high school, my chemistry teacher asked me to take over her lecture one day and to explain to my classmates the helical structure of DNA. I relished the opportunity, and, as I prepared my presentation, I identified many gaps in my own knowledge and sought to fill them, leading to (what I hope was) a more cogent lecture for the other students.

When I reached my senior year of college as a chemistry and mathematics major at Duke University, I was the only undergraduate asked to teach two chemistry laboratory courses, and there I truly discovered my love of teaching and a knack for communicating complex scientific ideas. One day, while teaching a general chemistry laboratory to a group of 20 first-year students, I became so energized in explaining a key concept that I grabbed the chalk and furiously wrote the idea on the board. My students dutifully copied what I'd written into their notebooks and returned to their experiments. Only then did I realize that, in my haste and enthusiasm, I'd written everything with my right hand—even though I'm a lefty. Somehow, although my writing was (more or less) legible, all of the lower-case letters "e" were reversed. (None of the students felt it necessary to inform me of this, for some reason!)

These experiences also revealed to me the tremendous satisfaction derived from actually seeing understanding spread across the face of a student or colleague when your explanation really "hits home". As a postdoctoral associate at the University of Texas, I once gave the *last* lecture on the program at a regional theoretical chemistry conference. The subject of the talk was artifactual symmetry breaking in molecular radicals, a rather technical and complicated topic, and the conclusions were unexpected to many in attendance. However, as I carefully walked my audience through a detailed explanation of our results, I could glean directly from their faces their gradual comprehension of the meaning behind the work. After my presentation was finished, the organizer of the conference generously invited me to give the *opening* talk of the same conference the next year. Since that experience, I have always viewed my conference presentations to professional scientists no differently than classroom lectures to undergraduate or graduate students: the goal is always to *teach*. Though the level of expertise and discourse may vary, one should always convey challenging scientific concepts with clarity and enthusiasm so that everyone will learn something new.

The need for clear communication and exposition of complex ideas is particularly important in my field of research: molecular quantum mechanics. My students and I develop advanced theoretical descriptions and computational simulations of the interaction of electromagnetic

radiation with chiral compounds—molecules with an inherent "handedness"—such as sugars, proteins, enzymes, and nearly all modern drugs. The concept of chirality, especially in compounds of importance in the human metabolism, has played a pivotal role in chemistry almost since the concept of the atom was introduced in the early 19th century. However, in spite of nearly two centuries of experience with chiral phenomena, the chemical community does not yet have sufficient grasp of the key relationship between molecular structure and the spectroscopic response of such compounds to make intuitive predictions thereof—that is, chemists do not yet *understand* chirality. One of the central goals of my research is to develop and convey such understanding to the community.

Mentorship plays a pivotal role in all aspects of my scientific life. My research is intimately connected to mentorship of both Ph.D. students and postdoctoral associates. Indeed, I view my students and postdocs as "fellow travelers" in scientific discovery, and their development as independent scientists is one of the most satisfying parts of a professor's career and a major component of my personal legacy. My Ph.D. adviser once told me to treat my graduate students as though they were my children, and my research group as a family. I took this advice to heart, and I give them as much of my time as I possibly can.

My field of molecular science is global, and thus its rapid advance towards the solution of modern Grand Challenges depends on broad collaborations spanning the international community. Much of my work has involved such collaborations with scientists in Norway, the U.K., France, Japan, China, Australia, India, Italy, Sweden, Denmark, the Netherlands, Germany, and more. Moreover, my efforts to effect improvements in the way molecular science is carried out—both in terms of research and education—have been global. For example, my development of online programming exercises designed to teach software development to quantum chemistry students reaches dozens of research groups both inside and outside of the U.S. The molecular response properties summer schools I have organized (with co-organizers from France, Norway, and Sweden) have attracted students from Europe and Asia, as well as the U.S., and my involvement in the European Summer School on quantum chemistry reaches students from around the world.

The vast majority of the software development in the molecular sciences is carried out by graduate students and postdoctoral researchers in chemistry and physics for whom the natural motivation is short-term scientific expediency—a "just get the physics working" approach—rather than establishing a foundation for the sustainable, long-term effort needed to address scientific Grand Challenges. This problem is magnified by a physical sciences culture in which the education of undergraduate and graduate students involves little to no exposure to modern software engineering tools and techniques. As a result, many research groups are forced to train their students in software development in an *ad hoc* manner. My establishment of the Molecular Sciences Software Institute (MolSSI) and its broad education and research mandates are specifically intended to overcome these obstacles. The MolSSI's Software Fellowship program has mentored 115 graduate students and postdocs across the U.S., and our Education Initiative has directly benefitted tens of thousands of students worldwide through our face-to-face and online education workshops and curricula.

My larger goal is to raise the quality of teaching, software engineering, and cutting-edge research across the global molecular sciences community in order to enable our field to address ever larger and more complex scientific problems. Bringing such a diverse and headstrong community together toward a common set of goals requires not only a deep understanding of the technical challenges we face, but also a personal understanding of the people themselves – and the mutual respect that a community leader needs to facilitate such change.

CURRICULUM VITAE—T. DANIEL CRAWFORD
http://www.crawford.chem.vt.edu

EDUCATION:

1992	Bachelor of Science in Chemistry (*cum laude*), Duke University
1996	Doctor of Philosophy in Theoretical Chemistry, University of Georgia

PROFESSIONAL APPOINTMENTS:

2019-present	University Distinguished Professor, Department of Chemistry, Virginia Tech
2016-present	Ethyl Chair Professor, Department of Chemistry, Virginia Tech
2009-2016	Professor, Department of Chemistry, Virginia Tech
2009	Visiting Professor, University of Oslo, Norway
2009	Visiting Professor, University of Tromsø, Norway
2005-2009	Associate Professor, Department of Chemistry, Virginia Tech
2000-2005	Assistant Professor, Department of Chemistry, Virginia Tech
1997-2000	Postdoctoral Fellow, Department of Chemistry, University of Texas

SELECTED HONORS and AWARDS:

2023	Cottrell Scholar STAR Award, Research Corp. for Science Advancement
2022	Elected Member, International Academy of Quantum Molecular Sciences
2022	Governing Board, World Assoc. of Theoretical and Computational Chemists
2019	University Distinguished Professor, Virginia Tech
2017	Peter C. Reilly Lecturer, U. Notre Dame
2016	Ethyl Corporation Professorship in Chemistry, Virginia Tech
2015	Fellow of the American Chemical Society
2012	Alumni Award for Excellence in Research, Virginia Tech
2005, 2012	James Viers Faculty Teaching Award, Virginia Tech
2010	Dirac Medal of the World Association of Theoretical and Computational Chemists “For the outstanding computational chemist in the world under the age of 40”
2008	John C. Schug Faculty Research Award, Virginia Tech
2005	Certificate of Teaching Excellence, Virginia Tech
2004	Young Investigator Award, International Journal of Quantum Chemistry
2003-2008	Cottrell Scholar Award, Research Corp. for Science Advancement
2002	National Science Foundation Early CAREER Award
2000	Research Innovation Award, Research Corp. for Science Advancement
2000	New Faculty Award, Camille and Henry Dreyfus Foundation
1993-1996	National Defense Science and Engineering Graduate Fellowship, U. Georgia
1992-1996	Fritz London Graduate Fellowship, U. Georgia
1992	Kenneth Gordon Fellowship for Advanced Independent Study, Duke Univ.

SELECTED PUBLICATIONS (155 TOTAL, H-INDEX=47, TOTAL CITATIONS=10,811):

1. T. D. Crawford, *Theor. Chem. Acc.*, 115, 227-245 (2006). Ab Initio Calculation of Molecular Chiroptical Properties. **(407 citations)**
2. T. D. Crawford, M. C. Tam, and M. L. Abrams, *J. Phys. Chem. A*, 111, 12057-12068 (2007). The Current State of *Ab Initio* Calculations of Optical Rotation and Circular Dichroism Spectra. **(280 citations)**
3. T. D. Crawford and H. F. Schaefer, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, 2000, Vol. 14, Chap. 2, pp. 33–136. An introduction to coupled cluster theory for computational chemists. **(987 citations)**

4. J. M. Turney, A. C. Simmonett, R. M. Parrish, E. G. Hohenstein, F. Evangelista, J. T. Fermann, B. J. Mintz, L. A. Burns, J. J. Wilke, M. L. Abrams, N. J. Russ, M. L. Leininger, C. L. Janssen, E. T. Seidl, W. D. Allen, H. F. Schaefer, R. A. King, E. F. Valeev, C. D. Sherrill, and T. D. Crawford, *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 2, 556-565 (2012). PSI4: An Open-Source Ab Initio Electronic Structure Program. **(1045 citations)**
5. R. M. Parrish, L. A. Burns, D. G. A. Smith, A. C. Simmonett, A. E. D. III, E. G. Hohenstein, U. Bozkaya, A. Y. Sokolov, R. D. Remigio, R. M. Richard, J. F. Gonthier, A. M. James, H. R. McAlexander, A. Kumar, M. Saitow, X. Wang, B. P. Pritchard, P. Verma, H. F. S. III, K. Patkowski, R. A. King, E. F. Valeev, F. A. Evangelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill, *J. Chem. Theory Comp.*, **13**, 3185-3197 (2017). Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. **(1100 citations)**

FUNDING RECORD:

- 28 research awards (19 as PI, 9 as co-PI) totaling $41.8M
- Diverse funding sources, including the National Science Foundation, Department of Energy, Department of Defense, Research Corporation for Science Advancement, NASA, Jeffress Memorial Trust, Camille & Henry Dreyfus Foundation
- Continuously funded by the National Science Foundation since 2001

TEACHING:

- Mentored 17 Ph.D. students (6 current), 12 postdoctoral associates, and 39 undergraduate researchers (3 current)
- Taught at all levels of the chemistry curriculum, from general chemistry to advanced undergraduate physical chemistry to graduate level courses
- One of the highest rated professors at Virginia Tech, with an overall student evaluation score of 5.78/6.00
- Recognitions: Viers Teaching Award (2005, 2012), Certificate of Teaching Excellence (2005), Favorite Faculty Award (student-nominated; multiple years)

SELECTED PROFESSIONAL SERVICE:

1. Deputy Editor, *Journal of Physical Chemistry A*, 2021-present; Senior Editor, *Journal of Physical Chemistry*, 2012-2020
2. Secretary/treasurer of the Physical Chemistry (PHYS) Division of the American Chemical Society, 2012-2017
3. Organizer/co-organizer of 13 conferences and symposia, including six ACS symposia and three major international meetings
4. Director of the Molecular Sciences Software Institute (MolSSI), dedicated to the advancement of computational chemistry software and to the education and training of the next generation of computational molecular scientists (molssi.org)
5. Board of Directors, International Society of Theoretical Chemical Physics, 2013-present
6. Currently serving on seven international Research Advisory Boards
7. Reviewer for dozens of journals, including *Science*, *Journal of the American Chemical Society*, *Nature Chemistry*, *Journal of Chemical Theory and Computation*, *Journal of Chemical Physics*, *Angewandte Chemie*, etc.
8. Reviewer for numerous funding agencies, including NSF, DOE, DOD, AFOSR, NSERC (Canada), *Centre Européen de Calcul Atomique et Moléculaire* (CECAM), Max Planck Society (Germany), etc.
9. Served as an external opponent for doctoral student defenses in Aarhus, Denmark, Trondheim, Norway, Stockholm, Sweden, Ghent, Belgium, and Copenhagen, Denmark

Letters of Support (Excerpted)

Letters from Virginia Tech Administration/Supervisors:

"Prof. Crawford's research stands at the cutting edge of molecular quantum mechanics and advances the role of both Virginia Tech and the commonwealth on the world's scientific stage…As an educator, Prof. Crawford is among Virginia Tech's finest. He has raised the bar in chemistry instruction from general chemistry to advanced graduate courses, and his students and colleagues alike consider him to be one of the most effective communicators in the university community. His efforts have also elevated the global profile of Virginia Tech through his more than 200 invited lectures in two dozen countries. In 2019, the university recognized Prof. Crawford's numerous contributions to science, education, the university community, and to his profession by awarding him the title of University Distinguished Professor – the most esteemed rank bestowed on only the top 1% of our faculty. Along with Virginia Tech's recognition of Prof. T. Daniel Crawford's scholarship, I believe he is also eminently deserving of a SCHEV Outstanding Faculty Award."

President Timothy D. Sands, Virginia Tech

"Prof. Crawford is a stellar scientist who has transformed Virginia Tech and is transforming the way computational scientists throughout the world approach software challenges. Crawford joined the Department of Chemistry at Virginia Tech in 2000 and, at the time of his arrival, he was immediately recognized as a future leader in the area of coupled-cluster calculations for solving problems in quantum mechanics...Crawford excels at everything he does, and I firmly believe that he will succeed in obtaining his ultimate goal `…to change fundamentally the software development enterprise–both education and culture–of the entire computational molecular sciences community.'"

Dr. Cyril R. Clarke, Executive Vice President and Provost, Virginia Tech

Letters from Professional Colleagues:

"Dr Crawford's pattern of sustained excellence in research and scholarship has led to his being recognized as one of the international leaders in theoretical and computational chemistry. He is an international leader in the design and implementation of efficient techniques for deriving chemically useful properties from coupled cluster calculations. His particular strength is chiroptical properties, such as optical rotation and circular dichroism, where he is the world leader. His pre-eminence has been recognized by numerous invitations to write review articles and to present lectures at international conferences. He is not only an excellent researcher, but also a gifted communicator who gives some of the clearest and best organized theoretical chemistry lectures that I have ever heard."

Prof. Peter M. W. Gill, University of Sydney, Australia

"Daniel is one of the most outstanding theoretical chemists of his generation, internationally recognized for his development of high-accuracy, yet computationally efficient, first-principles quantum mechanical methods for prediction of a wide variety of molecular properties, as well as for making the resulting programs readily available to the entire scientific community. In addition, he has earned a reputation as one of the field's clearest communicators, and his lectures are popular among students and established experts alike, as evident from his many invited lectures at conferences and universities worldwide…Professor Crawford has also made considerable efforts to distribute computational software freely to the entire scientific community, methodology developed by his research group and also that of others. The most ambitious step in this direction is the Molecular Sciences Software Institute, funded by a major grant from the National Science Foundation, that he organized and leads…This is a very ambitious undertaking, and I can think of no one who has a better chance at making it a success."

Prof. William H. Miller, U.C. Berkeley

"Prof. Crawford is one of the world's top experts on molecular properties and their quantum-mechanical description — in particular, the chiroptical properties of molecules. In spite of the ubiquity of chirality in chemistry and biology, the detailed relationship between molecular structure and chiral properties remains a mystery. Prof. Crawford has developed the computational tools to study such properties at the highest level of precision and applied these tools to elucidate the mechanism underlying optical activity and spectroscopic processes…Prof. Crawford is a superb speaker. While visiting Oslo in 2009, he gave tutorials on advanced quantum chemistry, demonstrating excellent pedagogical skills."

Prof. Trygve Helgaker, University of Oslo

Letters from Students:

"Prof. T. Daniel Crawford was the absolute best mentor I could have had in graduate school. I often say how rare it is for former students to have nothing but the highest praise for their Ph.D. advisors, but I am one of the fortunate ones who, after the years of stretching, pushing, and growing that graduate school entails, still admire Dr. Crawford more than ever... I knew then and still know now that he wants the best for me. While in grad school Dr. Crawford enabled my connections to my eventual post-doc advisor at NASA Ames. Later, he helped me navigate the path to getting a tenure- track job and even in moving to a more prestigious university. Without Dr. Crawford, I would be nowhere near where I am today…Dr. Crawford's humanity is his greatest strength, and it comes out in all of these areas."

Prof. Ryan C. Fortenberry, University of Mississippi

"My time at Virginia Tech was one of immense personal and professional growth much of which I attribute directly to Professor Crawford's comportment and the manner in which he guided his research group…Dr. Crawford treated members of the group as peers while simultaneously serving as our mentor. His approach to leadership set the tone in the group…In fact, we called ourselves the crawkids, our own play on his email address stemming from the sense of community we had in the group…Today, as a professor myself, I marvel at the thoroughness with which he prepared for each and every class meeting. I recall him telling us several times that he had stayed up all night preparing for our special topics course in advanced electronic structure theory as he was literally writing the text for the class as we were taking it."

Prof. Taylor J. Mach, Concordia University

"After just one meeting in Professor Crawford's office hours, my trepidation [about studying chemistry] began to fade, and shortly after, Professor Crawford's office hours became a staple of my weekly routine, an inspiration for my love of learning, and a foundation for my Hokie chemistry family…Professor Crawford's enthusiasm for teaching spilled over into the classroom and he was able to enrapture students with his energy and occasional tangents…Inspiring education and fostering relationships are the two key facets that made Professor Crawford my all-time favorite teacher and I consider myself one of the luckiest students to have had multiple courses with him…Professor Crawford taught me how to think conceptually and approach science with a more inquisitive nature. I would not be where I am today without his inspiration to push boundaries in my education and think innovatively."

Olivia Renaldo, Pharmacy Resident, Children's Hospital of Philadelphia

Letter from a Community Leader:

"In addition to attaining academia's highest accolades as a UDP, Daniel Crawford makes time to serve others as a community-builder at every level: Blacksburg, Virginia, America, our world. Having collaborated with Daniel for two decades at our local parish, I have watched with amazement how naturally Daniel volunteers and undertakes many charitable, humble and thankless tasks that make a difference in people's lives…Daniel has served as a member of our Parish Advisory Council, lector, liturgical trainer, and homeless shelter driver/coordinator…In addition to his intellectual brilliance, Daniel is grounded in a life of altruistic service. What more can we ask of a fellow human?"

Rev. Mike W. Ellerbrock, Ph.D., Catholic Deacon and Virginia Tech Professor