

Christopher J. Cramer

Date of birth: September 23, 1961

Curriculum Vitae

(as of September 19, 2021)

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EDUCATION

Doctor of Philosophy, Chemistry, University of Illinois, Urbana-Champaign, 1988.
Artium Baccalaurei, summa cum laude, Washington University, St. Louis, Missouri,
Mathematics and Chemistry, 1983.

PROFESSIONAL EXPERIENCE

Underwriters Laboratories Inc. Senior Vice President and Chief Research Officer	2021–present
BioMADE Manufacturing Innovation Institute Board of Directors, Member	2021–present
University of Minnesota, Minneapolis–St. Paul Vice President for Research	2018–2021
College of Science and Engineering, Associate Dean for Research and Planning	2018
Associate Dean for Academic Affairs	2013–2018
Distinguished McKnight and University Teaching Professor	2000–2021
Associate Professor of Chemistry, Chemical Physics, and Scientific Computation	1996–2000
Assistant Professor of Chemistry and Chemical Physics	1992–1996
Director, Center for Charge Transfer and Charge Transport in Photoactivated Systems (DOE SciDAC)	2012–2017
Fellow, Big Ten Academic Alliance Academic Leadership Program	2013–2014
Faculty Liaison for eLearning Initiatives, Office of the Senior Vice President for Academic Affairs and Provost	2012–2013
Professeur Invité, University of Geneva, Switzerland	2007–2008
Visiting Professor, University of Barcelona, Catalonia, Spain	2000–2001
Hubert H. Humphrey Institute Policy Fellow	1996
Officer, United States Army, Chemical Corps	1988–1992

SELECTED AWARDS AND HONORS

American Chemical Society Arthur C. Cope Scholar Award	2021
Labex MiChem Professeur Invité, Sorbonne Universités, Paris	2015
George W. Taylor Distinguished Service Award	2013
University of Minnesota Morse–Alumni Undergraduate Teaching Award	2011
Fellow of the American Chemical Society	2010
Elmore H. Northey Chair, Chemistry	2009–2014

University of Minnesota Inventor Recognition Award	2005, 2008
University of Minnesota Postbaccalaureate, Graduate, and Professional Education Award	2005
John Simon Guggenheim Fellowship	2000
George W. Taylor Distinguished Research Award	1999
Alfred P. Sloan Research Fellow	1996
8th Annual Army Materiel Command Outstanding Research Award	1992
Arthur S. Flemming Award	1991
Army Research and Development Achievement Award	1991
Army Special Act Award in Recognition of Research Excellence	1991
National Science Foundation Graduate Fellow	1984

SELECTED ADMINISTRATIVE EXPERIENCE

Leadership: Currently serving as Senior Vice President and Chief Research Officer for Underwriters Laboratories Inc., a 501(c)(3) non-profit corporation dedicated to advancing public safety through the discovery and application of scientific knowledge. The CRO provides strategic vision and resources to support the work of established research institutes, and actively engages in launching and stewarding new initiatives that address safety-science concerns associated with emerging technologies. The CRO is a key member of the organization's executive leadership team, and serves as the technical spokesperson to public and private external stakeholders, helping to foster collaborative research interactions, and also to drive the development of voluntary standards adoptions and public policy.

Previously served as Vice President for Research (VPR), having responsibility for providing vision and leadership to the University of Minnesota's research programs, which expend \$1+B per year. As VPR, served as the institution's chief research officer, overseeing research support and services at the University's five campuses, providing guidance to individual researchers, and managing the systemwide research enterprise; as VPR, also served as a member of the President's Senior Leadership Team and Cabinet. As VPR, helped develop innovative approaches to enhance research productivity and encourage university-industry partnerships; coordinated multidisciplinary research programs; and represented the University of Minnesota to local, regional, national, and international constituencies, as well as to federal and other funding agencies. Finally, as VPR also oversaw the responsible planning, stewardship, management, and accountability of all fiscal, capital, and human resources of administrative and academic units that reported to the OVPR, which comprised approximately 750 FTE staff positions and an annual budget of ~\$150M.

Also previously served as Chair of, and Councilor representing, a 5,000-member division of the American Chemical Society, working with a divisional executive board and national organizational staff to develop, fund, implement, and manage programmatic and membership activities. Previously served as Chair of faculty governance at the University of Minnesota, working with staff and other governance bodies to contribute to University shared governance. Previously served for 14 years as Editor-in-Chief of a scientific journal, charged with budgetary, content, and thematic decisions, managing relevant staff. History as principal investigator for single- and multi-investigator research awards totaling in excess of \$15M over 27 years including Directorship of a multi-institution Scientific Discovery through Advanced Computing (SciDAC) application project.

Program Management: Served as Associate Dean for Research and Planning in the University of Minnesota's College of Science and Engineering, with oversight of research and compliance activities related to sponsored projects totalling ~\$140M per year. Also served as Associate Dean for Academic Affairs, with responsibility for (i) oversight of faculty hiring, promotion, and tenure within the College, awards, diversity programs, salary equity, sabbaticals and leaves, governance activities, and a variety of other miscellaneous

management and liaison activities and (ii) oversight and support of graduate education programs within the College serving ~2,500 graduate students and administration of \$2.4M per year associated annual budget.

Served as Faculty Liaison for eLearning Initiatives in the Office of the Senior Vice President for Academic Affairs and Provost with institution-wide responsibilities for development and enhancement of digital curricular strategies and materials, including online learning, Massive Open Online Courses (MOOCs), and management of a \$500K initiative to enhance undergraduate programs using digital technology.

Served as Director of Graduate Studies for the University of Minnesota's largest Ph.D. program, Chemistry, managing associated budget and staff. Served as Director of Undergraduate Studies for Chemistry, managing associated budget and staff. Continuous management of a Chemistry/Chemical Physics research group having a typical annual budget of six figures and multiple direct reports.

Diversity and Inclusion: Working with internal partners to ensure Underwriters Laboratories maintains a culture where every staff member feels valued and empowered, recognizing that decisions made with the incorporation of diverse viewpoints and experiences are inevitably more robust than otherwise. Working with external partners, including especially partner institutions of higher education and the GEM Fellowship Program, to foster the success of junior researchers from historically underrepresented populations as they embark upon and launch their professional careers.

Previously managed recurring lecture and networking events designed to support underrepresented scholars in the College of Science and Engineering; encouraged and fostered the success of self-organizing student groups focused on climate and diversity. Directed targeting of graduate education funding to improve diversity in recruitment and retention. Led faculty-governance component of University of Minnesota Gender-Related Faculty Salary Analysis Working Group. Regular attendee and organizer of events devoted to increasing diversity, in STEM disciplines in particular. Served as Chair of Chemistry's faculty search committee from 2010–2012 and implemented a strategy that led to approx. 50% of interviewed candidates being women or underrepresented minorities.

Public Engagement: Spokesperson to public and private groups engaging with Underwriters Laboratories Inc., to include entities charged with informing governmental policy. Contributor to civic leadership in the greater Chicago area. An episodic expert for news media querying the American Chemical Society and also active in various social media.

As VPR for the University of Minnesota, provided testimony before the Minnesota State House and Senate Higher Education Committees. Author and quoted source for commentaries and articles in the *Minneapolis Star-Tribune*, *St. Paul Pioneer Press*, and other newspapers and higher education journals.

Military: Exercised staff and command responsibilities in administrative and tactical operations, including armed combat (Operations Desert Shield and Desert Storm).

SCHOLARLY RESEARCH CONTRIBUTIONS

Modeling catalysis, including the exploitation of metal-organic frameworks, to advance sustainable chemistry and chemical processes

Molecular and material phenomena associated with solar energy devices and semiconductors

Theoretical characterization of small-molecule activation at transition-metal centers

Modeling remediation of environmental contaminants and chemical warfare agents

Development and application of condensed-phase quantum chemical models

RESEARCH SUPPORT

Summary: From 1992–2021, approx. \$20M in individual and small-team grant support from, inter alia, the U.S. Army Research Office, the National Science Foundation, the Department of Energy, the Defense Threat Reduction Agency, the U.S. Army Engineering Research & Development Center, the Office of Naval Research, the State of Minnesota, the U.S.

Environmental Protection Agency, the National Institute of Standards and Technology, Silicon Graphics, Cray, and Kodak Inc.

TECHNOLOGY TRANSFER

- Licensed Software, *MNSOL Database*, University of Minnesota Office for Technology Commercialization 2008
- Licensed Software, *AMSOL*, University of Minnesota Office for Technology Commercialization 2005

RESEARCH MENTORSHIP

University of Minnesota, 1992-2021

- Postdoctoral Associates: 39 (1 current)
- Graduate Students: 31 doctoral students (1 current); 7 masters students
- Undergraduate Students: 71 (a large majority of whom went on to pursue post-graduate studies in doctoral or professional programs)
- High-school students: 4 (who went on to attend Stanford, MIT (2), and the University of Illinois)
- Visiting scientists/faculty: 28

PUBLICATIONS (64,000+ citations, *h* index = 106, Google Scholar)

Books, Authored

1. Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models*, Wiley: Chichester, 2002.
2. Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models, 2nd Edition*, Wiley: Chichester, 2004.

Book Series, Edited

1. *Highlights in Theoretical Chemistry*, Vols. 1–11, Cramer, C. J.; Truhlar, D. G., Series Eds., Springer Verlag: Berlin Heidelberg, 2012–2016.

Recent Journal Articles/Refereed Book Chapters, Authored

494. Pratik, S. M.; Gagliardi, L.; Cramer, C. J. "Boosting Photoelectric Conductivity in Porphyrin-based MOFs Incorporating C₆₀" *J. Phys. Chem. C* **2020**, *124*, 1878 (doi:10.1021/acs.jpcc.9b10834).
495. Kim, H. J.; Reddi, Y.; Cramer, C. J.; Hillmyer, M. A.; Ellison, C. J. "Readily Degradable Aromatic Polyesters from Salicylic Acid" *ACS Macro Lett.* **2020**, *9*, 96 (doi:10.1021/acsmacrolett.9b00890).
496. Luke, A. M.; Peterson, A.; Chiniforush, S.; Mandal, M.; Popowski, Y.; Sajjad, H.; Bouchey, C.; Shopov, D. Y.; Graziano, B.; Yao, L. J.; Cramer, C. J.; Reineke, T. M.; Tolman, W. B. "Mechanism of Stereocontrol in Polymerization of *rac*-Lactide by Aluminum Complexes Supported by Indolide-Imine Ligands" *Macromolecules* **2020**, *53*, 1809 (doi:10.1021/acs.macromol.0c00092).
497. Noland, W. E.; Kumar, H. V.; Reddi, Y.; Cramer, C. J.; Novikov, A. V.; Kim, H.; Zhu, Y.; Chin, Y. C.; Zhou, Y.; Radakovic, P.; Uprety, A.; Xie, J.; Flick, G. C. "Diels–Alder/Ene Reactivities of 2-(1'-Cycloalkenyl)thiophenes and 2-(1'-Cycloalkenyl)benzo[*b*]thiophenes with *N*-Phenylmaleimides: Role of Cycloalkene Ring Size on Benzothiophene and Dibenzothiophene Product Distributions" *J. Org. Chem.* **2020**, *85*, 5265 (doi:10.1021/acs.joc.9b03363).
498. Aprà, E.; Bylaska, E. J.; de Jong, W. A.; Govind, N.; Kowalski, K.; Straatsma, T. P.; Valiev, M.; van Dam, H. J. J.; Alexeev, Y.; Anchell, J.; Anisimov, V.; Aquino, F.; Atta-Fynn, R.; Autschbach, J.; Bauman, N. P.; Bernholdt, D. E.; Bhaskaran-Nair, K.; Bogatko, S.; Borowski,

- P.; Boschen, J.; Brabec, J.; Cauët, E.; Chen, Y.; Chuev, G. N.; Cramer, C. J.; Daily, J.; Deegan, M. J. O.; Dunning, T. H., Jr.; Dupuis, M.; Dyall, K. G.; Fann, G. I.; Fischer, S. A.; Fonari, A.; Früchtl, H.; Gagliardi, L.; Garza, J.; Gawande, N.; Ghosh, S.; Glaesemann, K.; Götz, A. W.; Hammond, J.; Helms, V.; Hermes, E.; Hirata, S.; Jacquelin, M.; Jensen, L.; Johnson, B. G.; Jonsson, H.; Kendall, R. A.; Klemm, M.; Kobayashi, R.; Krishnamoorthy, S.; Krishnan, M.; Lin, Z.; Lins, R. D.; Littlefield, R. J.; Logsdail, A.; Lopata, K.; Ma, W.; Marenich, A.; Martin del Campo, J.; Mejia-Rodriguez, D.; Moore, J. E.; Mullin, J. M.; Nichols, J. A.; Nichols, P.; Nieplocha, J.; Otero de la Roza, A.; Palmer, B.; Panyala, A.; Pirojsirikul, T.; Peng, B.; Peverati, R.; Pittner, J.; Pollack, L.; Richard, R. M.; Sadayappan, P.; Silverstein, D.; Smith, D. M. A.; Soares, T. A.; Song, D.; Swart, M.; Taylor, H. L.; Thomas, G.; Tipparaju, V.; Truhlar, D. G.; Tsemekhman, K.; Van Voorhis, T.; Vázquez-Mayagoitia, Á.; Verma, P.; Villa, O.; Vishnu, A.; Vogiatzis, K. D.; Wang, D.; Weare, J. H.; Williamson, M. J.; Windus, T. L.; Wolinski, K.; Wong, A. T.; Wu, Q.; Yang, C.; Yu, Q.; Zacharias, M.; Zhang, Z.; Zhao, Y.; Harrison, R. J. “NWChem: Past, Present, and Future” *J. Chem. Phys.* **2020**, *152*, 184102 (doi:10.1063/5.0004997).
499. Singh, S. K.; Cramer, C. J.; Gagliardi, L. “Correlating Electronic Structure and Magnetic Anisotropy in Actinide Complexes [An(COT)₂], An^{III/IV} = U, Np, and Pu” *Inorg. Chem.* **2020**, *59*, 6815 (doi:10.1021/acs.inorgchem.0c00105).
500. Flemming, H.; Engelage, E.; Cramer, C. J.; Huber, S. M. “Hypervalent Iodine(III) Compounds as Biaxial Halogen Bond Donors” *J. Am. Chem. Soc.* **2020**, *142*, 8633 (doi:10.1021/jacs.9b13309).
501. Suh, S.-E.; Chen, S.-J.; Mandal, M.; Guzei, I. A.; Cramer, C. J.; Stahl, S. S. “Site-Selective Copper-Catalyzed Azidation of Benzylic C–H Bonds” *J. Am. Chem. Soc.* **2020**, *142*, 11388 (doi:10.1021/jacs.0c05362).
502. Pratik, S. M.; Gagliardi, L.; Cramer, C. J. “Engineering High Electrical Conductivity in Stable Zirconium-based PCN-222 MOFs with Permanent Mesoporosity” *Chem. Mater.* **2020**, *32*, 6137 (doi:10.1021/acs.chemmater.0c01847).
503. Mendonca, M. L.; Ray, D.; Cramer, C. J.; Snurr, R. Q. “Exploring the Effects of Node Topology, Connectivity, and Metal Identity on the Binding of Nerve Agents and Their Hydrolysis Products in Metal–Organic Frameworks” *ACS Appl. Mater. Interfaces* **2020**, *12*, 35657 (doi:10.1021/acsami.0c08417).
504. Wang, X.; Zhang, X.; Pandharkar, R. U.; Lyu, J.; Ray, D.; Yang, Y.; Kato, S.; Liu, J.; Wasson, M. C.; Islamoglu, T.; Li, Z.; Hupp, J. T.; Cramer, C. J.; Gagliardi, L.; Farha, O. K. “Insights into the Structure-Activity Relationships in Metal–Organic Frameworks-Supported Nickel Catalysts for Ethylene Hydrogenation” *ACS Catal.* **2020**, *10*, 8995 (doi:10.1021/acscatal.0c01844).
505. Shao, H.; Reddi, Y.; Cramer, C. J. “Modeling the mechanism of CO₂/cyclohexene oxide copolymerization catalyzed by chiral zinc β-diiminates: factors affecting reactivity and isotacticity” *ACS Catal.* **2020**, *10*, 8870 (doi:10.1021/acscatal.0c02299).
506. Mandal, M.; Cramer, C. J.; Truhlar, D. G.; Sauer, J.; Gagliardi, L. “Structure and Reactivity of Single-Site Vanadium Catalysts Supported on Metal–Organic Frameworks” *ACS Catal.* **2020**, *10*, 10051 (doi:10.1021/acscatal.0c02300).
507. Song, H.; Fischer, S. A.; Zhang, Y.; Cramer, C. J.; Mukamel, S.; Govind, N.; Tretiak, S. “First Principles Non-Adiabatic Excited-State Molecular Dynamics in NWChem” *J. Chem. Theor. Comput.* **2020**, *16*, 6418 (doi:10.1021/acs.jctc.0c00295).
508. Zhu, Y.; Zheng, J.; Ye, J.; Cui, Y.; Koh, K.; Kovarik, L.; Camaioni, D. M.; Fulton, J.; Truhlar, D. G.; Neurock, M.; Cramer, C. J.; Gutiérrez, O. Y.; Lercher, J. A. “Copper-zirconia interfaces in UiO-66 enable selective catalytic hydrogenation of CO₂ to methanol” *Nature Commun.* **2020**, *11*, 5849 (doi:10.1038/s41467-020-19438-w).
509. Varner, T. P.; Teator, A. J.; Reddi, Y.; Jacky, P. E.; Cramer, C. J.; Leibfarth, F. A. “Mechanistic Insight into the Stereoselective Cationic Polymerization of Vinyl Ethers” *J. Am. Chem. Soc.* **2020**, *142*, 17175 (doi:10.1021/jacs.0c08254).
510. Hackler, R. A.; Pandharkar, R.; Ferrandon, M. S.; Kim, I. S.; Vermeulen, N. A.; Gallington, L. C.; Chapman, K. W.; Farha, O. K.; Cramer, C. J.; Sauer, J.; Gagliardi, L.; Martinson, A. B.

- F.; Delferro, M. "Isomerization and Selective Hydrogenation of Propyne: Screening of Metal-Organic Frameworks Modified by Atomic Layer Deposition" *J. Am. Chem. Soc.* **2020**, *142*, 20380 (doi:10.1021/jacs.0c08641).
511. Vitillo, J. G.; Lu, C. C.; Cramer, C. J.; Bhan, A.; Gagliardi, L. "Influence of first and second coordination environment on structural Fe(II) sites in MIL-101 for C-H bond activation in methane" *ACS Catal.* **2021**, *11*, 579 (doi:10.1021/acscatal.0c03906).
512. Ray, D.; Goswami, S.; Duan, J.; Hupp, J. T.; Cramer, C. J.; Gagliardi, L. "Tuning the Conductivity of Hexa-Zirconium(IV) Metal-Organic Framework by Encapsulating Heterofullerenes" *Chem. Mater.* **2021**, *33*, 1182 (doi:10.1021/acs.chemmater.0c03855).
513. Pandharkar, R.; Hermes, M. R.; Cramer, C. J.; Truhlar, D. G.; Gagliardi, L. "Localized active space pair-density functional theory" *J. Chem. Theor. Comput.* **2021**, *17*, 2843.
514. Gagliardi, L.; Cramer, C. J. "Modeling Metal-Organic Frameworks and Other Functional Materials with Electronic Structure Theory" in *COMPUTATIONAL MODELING: From Chemistry to Materials to Biology: Proceedings of the 25th Solvay Conference on Chemistry*, Wüthrich, K., Weckhuysen, B.; Rongy, L., De Wit, A., Eds., World Scientific, Singapore, 2021; pp. 87-90.
515. Epifanovsky, E., Gilbert, A. T. B., Feng, X., Lee, J., Mao, Y., Mardirossian, N., Pokhilko, P., White, A. F., Coons, M. P., Dempwolff, A. L., Gan, Z., Hait, D., Horn, P. R., Jacobson, L. D., Kaliman, I., Kussmann, J., Lange, A. W., Lao, K. U., Levine, D. S., Liu, J., McKenzie, S. C., Morrison, A. F., Nanda, K. D., Plasser, F., Rehn, D. R., Vidal, M. L., You, Z.-Q., Zhu, Y., Alam, B., Albrecht, B. J., Aldossary, A., Alguire, E., Andersen, J. H., Athavale, V., Barton, D., Begam, K., Behn, A., Bellonzi, N., Bernard, Y. A., Berquist, E. J., Burton, H. G. A., Carreras, A., Carter-Fenk, K., Chakraborty, R., Chien, A. D., Closser, K. D., Cofer-Shabica, V., Dasgupta, S., Wergifosse, M. d., Deng, J., Diedenhofen, M., Do, H., Ehlert, S., Fang, P.-T., Fatehi, S., Feng, Q., Friedhoff, T., Gayvert, J., Ge, Q., Gidofalvi, G., Goldey, M., Gomes, J., González-Espinoza, C. E., Gulania, S., Gunina, A. O., Hanson-Heine, M. W. D., Harbach, P. H. P., Hauser, A., Herbst, M. F., Vera, M. H., Hodecker, M., Holden, Z. C., Houck, S., Huang, X., Hui, K., Huynh, B. C., Ivanov, M., Jász, Á., Ji, H., Jiang, H., Kaduk, B., Kähler, S., Khistyayev, K., Kim, J., Kis, G., Klunzinger, P., Koczor-Benda, Z., Koh, J. H., Kosenkov, D., Koulias, L., Kowalczyk, T., Krauter, C. M., Kue, K., Kunitsa, A., Kus, T., Ladjánszki, I., Landau, A., Lawler, K. V., Lefrancois, D., Lehtola, S., Li, R. R., Li, Y.-P., Liang, J., Liebenthal, M., Lin, H.-H., Lin, Y.-S., Liu, F., Liu, K.-Y., Loipersberger, M., Luenser, A., Manjanath, A., Manohar, P., Mansoor, E., Manzer, S. F., Mao, S.-P., Marenich, A. V., Markovich, T., Mason, S., Maurer, S. A., McLaughlin, P. F., Menger, M. F. S. J., Mewes, J.-M., Mewes, S. A., Morgante, P., Mullinax, J. W., Oosterbaan, K. J., Paran, G., Paul, A. C., Paul, S. K., Pavošević, F., Pei, Z., Prager, S., Proynov, E. I., Rák, Á., Ramos-Cordoba, E., Rana, B., Rask, A. E., Rettig, A., Richard, R. M., Rob, F., Rossomme, E., Scheele, T., Scheurer, M., Schneider, M., Sergueev, N., Sharada, S. M., Skomorowski, W., Small, D. W., Stein, C. J., Su, Y.-C., Sundstrom, E. J., Tao, Z., Thirman, J., Tornai, G. J., Tsuchimochi, T., Tubman, N. M., Veccham, S. P., Vydrov, O., Wenzel, J., Witte, J., Yamada, A., Yao, K., Yeganeh, S., Yost, S. R., Zech, A., Zhang, I. Y., Zhang, X., Zhang, Y., Zuev, D., Aspuru-Guzik, A., Bell, A. T., Besley, N. A., Bravaya, K. B., Brooks, B. R., Casanova, D., Chai, J.-D., Coriani, S., Cramer, C. J., Cserey, G., DePrince III, A. E., DiStasio Jr., R. A., Dreuw, A., Dunietz, B. D., Furlani, T. R., Goddard III, W. A., Hammes-Schiffer, S., Head-Gordon, T., Hehre, W. J., Hsu, C.-P., Jagau, T.-C., Jung, Y., Klamt, A., Kong, J., Lambrecht, D. S., Liang, W., Mayhall, N. J., McCurdy, C. W., Neaton, J. B., Ochsenfeld, C., Parkhill, J. A., Peverati, R., Rassolov, V. A., Shao, Y., Slipchenko, L. V., Stauch, T., Steele, R. P., Subotnik, J. E., Thom, A. J. W., Tkatchenko, A., Truhlar, D. G., Van Voorhis, T., Wesolowski, T. A., Whaley, K. B., Woodcock III, H. L., Zimmerman, P. M., Faraji, S., Gill, P. M. W., Head-Gordon, M., Herbert, J. M. and Krylov, A. I. "Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package" *J. Chem. Phys.* **2021**, *155*, 084801.