Faculty Position in Computational Chemistry / AI-Driven Drug Discovery (Open Rank)
University of Virginia
Charlottesville, Virginia

THE SEARCH

The Department of Chemistry in the College and Graduate School of Arts & Sciences, in collaboration with the Paul and Diane Manning Institute of Biotechnology at the University of Virginia (UVA), invites applications and nominations for a tenured faculty appointment in Computational Chemistry with a focus on molecular design and drug discovery. Depending on experience and interest, the successful candidate will have the opportunity to head a collaborative cohort helping to shape future concepts in AI Drug Discovery at the Manning Institute.

As a faculty member, the successful candidate will develop and lead an innovative, externally funded research program that advances computational methods for the discovery and design of functional molecules, in areas such as AI-driven drug discovery, generative modeling, molecular modeling, virtual screening, and predictive ADME/toxicity modeling. This faculty member will contribute to UVA Chemistry's undergraduate and graduate educational mission and play a key role in mentoring graduate students and postdoctoral scholars to help shape new educational and training opportunities that connect graduate education with the Manning Institute's biotechnology and translational research mission. The department is particularly interested in researchers whose computational work is closely integrated with experimental validation and translational applications. As part of the Manning Institute, the candidate will build AI and computational drug discovery capacity that supports translational programs across the University. The leadership role potentially carries strategic responsibility beyond the candidate's own laboratory, including shaping the Institute's long-term scientific direction and may include leading faculty and staff recruitment efforts, guiding budget and resource allocation decisions, and setting strategic priorities across the Manning Institute's portfolio of biotechnology programs and investments.

THE UNIVERSITY OF VIRGINIA

The University of Virginia was founded by Thomas Jefferson in 1819 to advance human knowledge, educate leaders, and cultivate an informed citizenry. Today, UVA encompasses twelve schools in Charlottesville, the College at Wise in Southwest Virginia, and UVA Northern Virginia and is supported by a global network of more than 250,000 alumni. Students represent virtually every state in the nation and nearly 100 countries. One of the largest employers in central Virginia, the University employs nearly 34,000 people, including approximately 11,000 faculty and staff and 10,000 employees across UVA Health. With a strong financial position, a reputation for academic excellence, and a longstanding commitment to access and affordability, UVA is consistently ranked among the nation's leading public universities. The University's strategic plan, *A Great and Good University*, guides its future through a focus on strengthening institutional excellence, cultivating a vibrant academic community, advancing research and discovery, and expanding service and societal impact.

As a Carnegie R1 institution, research, discovery, and innovation are central to UVA's mission and impact. The University maintains strong partnerships with federal and state agencies, private foundations, and leading companies across a wide range of industries. In 2024-25, UVA received $570 million in sponsored research awards from all sources and reported $829 million in annual research and development expenditures. The University's researchers have generated hundreds of invention disclosures and patents in recent years, supported by the Licensing & Ventures Group, which helps bring discoveries to market and contributes to a thriving regional innovation ecosystem.

Complementing this research enterprise is UVA Health, a renowned academic health system comprising the UVA Medical Center, UVA Community Health, the School of Medicine, School of Nursing, University of Virginia Physicians Group, Claude Moore Health Sciences Library, and an NCI-designated Comprehensive Cancer Center, along with a network of strategic partnerships across the Commonwealth. Founded in 1825 as the nation's tenth medical school, the School of Medicine anchors a health system committed to advancing outstanding patient care, educating future health professionals, and discovering new and better ways to treat disease. As the Commonwealth continues to invest in pharmaceutical and biotechnology development, UVA and UVA Health are helping shape a growing life sciences ecosystem through investments in research infrastructure, commercialization, and translational science, including the Paul and Diane Manning Institute of Biotechnology. These assets reflect UVA’s commitment to connecting fundamental discovery with clinical impact, educating future leaders, and contributing to the health and economic vitality of communities across Virginia in ways that embody the University’s aspiration to be a force for great and good.

More information about UVA can be found here: https://www.virginia.edu/

THE DEPARTMENT OF CHEMISTRY

UVA’s Department of Chemistry is a highly collaborative and interdisciplinary research community within the College and Graduate School of Arts & Sciences. The department is home to 33 faculty members,

approximately 130 graduate students, and 21 professional research staff, and offers robust undergraduate and graduate programs that pair the resources of a leading research university with a close-knit scholarly environment.

Research spans analytical, biological, inorganic, organic, and physical chemistry, with particular strengths at the intersections of chemistry with biology, materials science, computation, and energy. Interdisciplinary research is a hallmark of the department, supported by collaborative centers and programs that bring together expertise from across the University. These efforts span areas from catalysis and sustainable energy to molecular and biophysical science, nanoscale research, and atomic and molecular science, and foster collaboration across Arts & Sciences, Engineering, Medicine, and Data Science.

UVA continues to invest in the department's research and educational environment, including a recent $100 million renovation of the Chemistry building that provides modern facilities for research and teaching. The department's interdisciplinary culture is complemented by broader university strengths in data science, artificial intelligence, and advanced research computing. Connections with the School of Data Science provide opportunities for collaboration in artificial intelligence and machine learning and access to research computing and data analytics infrastructure, while partnerships with the Paul and Diane Manning Institute of Biotechnology, UVA Comprehensive Cancer Center, and researchers across the biomedical sciences create avenues for computational discoveries to inform experimental and translational research. These connections create a distinctive research environment that brings computational innovation, molecular discovery, and human health into closer alignment.

More information about the Department can be found here: https://chemistry.as.virginia.edu/

THE PAUL AND DIANE MANNING INSTITUTE OF BIOTECHNOLOGY

The Paul and Diane Manning Institute of Biotechnology was established in 2023 through a $100 million gift from Paul and Diane Manning. Together with significant investments from the University and the Commonwealth of Virginia, the initiative represents a $350 million commitment to advancing biomedical research and accelerating the translation of scientific discoveries into new treatments for patients.

The Manning Institute is focused on developing new cellular, gene, and immunotherapies and building the infrastructure needed to advance promising discoveries toward clinical use. Building on UVA's existing strengths in biotechnology and biomedical research, the Institute is creating a translational ecosystem in which fundamental discoveries are advanced through the full lifecycle from early discovery through clinical trials, manufacturing, and commercialization. Under the leadership of Executive Director Mark Esser, the Manning Institute is bringing together researchers from across Arts & Sciences, Medicine, Engineering, Data Science, and UVA Health to build a highly collaborative ecosystem to accelerate the translation of scientific discoveries into life-changing therapies. The Institute will concentrate these efforts in areas where UVA has established strengths, including oncology, immunology, neurological disease,

cardiovascular and metabolic disorders, and infectious diseases with an emphasis on developing innovative approaches to address rare and genetic disorders.

At the center of this effort will be a new 350,000-square-foot facility at UVA's Fontaine Research Park. While the Institute's new facility is under construction (expected to open in late 2027), UVA is actively recruiting faculty, developing scientific programs, and building collaborative research capacity in advance of its opening. Designed to support the Institute's work from discovery through clinical translation, the facility will bring together advanced research laboratories, core facilities, a vivarium, cGMP manufacturing capabilities, and patient-care space under one roof. These resources will enable researchers to produce gene and cell therapies at clinical-trial scale, a crucial step toward FDA approval. UVA is also developing a statewide clinical trials network to expand access to new treatments as they are developed and tested.

Beyond its research mission, the Manning Institute is designed to extend the impact of UVA's work beyond the University through new medicines, biotechnology ventures, industry partnerships, and talent development. Stronger connections among researchers, industry partners, and entrepreneurs will support the development and commercialization of new medicines while creating opportunities for new biotechnology companies to emerge from UVA research. The Institute will also help train the next generation of biotechnology leaders and contribute to the growth of Virginia's biotechnology sector, including efforts to attract new companies, investment, and high-quality jobs to the Commonwealth.

More information about the Manning Institute can be found here: https://manninginstitute.virginia.edu/

ROLE & QUALIFICATIONS

The successful faculty candidate will establish and lead an innovative, externally funded research program in computational chemistry focused on molecular design and drug discovery and engage in interdisciplinary collaborations spanning chemistry, data science, engineering, and the biomedical sciences. This faculty member will contribute to UVA's undergraduate and graduate educational mission and play a key role in mentoring graduate students and postdoctoral scholars to help shape new educational and training opportunities that connect graduate education with the Manning Institute's biotechnology and translational research mission.

Candidates must hold a Ph.D. in Chemistry, Computational Science, or a closely related field and demonstrate a strong record of scholarship. The successful candidate will bring expertise in developing computational methods for the discovery and design of functional molecules. Beyond scientific excellence, UVA seeks a collaborative and entrepreneurial scholar who thrives in building partnerships across institutional boundaries and who is excited by the opportunity to help develop a growing research enterprise. Appointment rank is open and will be commensurate with the successful candidate's qualifications and experience. Candidates with a record of research leadership comparable to that expected of a tenured faculty appointment, including experiences gained in industry or other non-academic research settings, are encouraged to apply.

APPLICATIONS, INQUIRIES, AND NOMINATIONS

Screening of complete applications will begin immediately and continue until the completion of the search process. Applications should include a cover letter, curriculum vitae, research statement, teaching statement, and contact information for three references. Materials should be submitted via the Isaacson, Miller website: https://www.imsearch.com/open-searches/university-virginia/faculty-computational-chemistryai-driven-drug-discovery.

Micah Pierce, Partner
Damla Williams, Senior Associate
Marlyn Desire, Senior Search Coordinator
Isaacson, Miller

The University of Virginia is an Equal Opportunity/Affirmative Action employer and welcomes applications from women, minorities, veterans, and persons with disabilities.

This document has been prepared based on the information provided by the University of Virginia. The material presented in this leadership profile should be relied on for informational purposes only. While every effort has been made to ensure the accuracy of this information, the original source documents and information provided by the University of Virginia would supersede any conflicting information in this document.