Leopoldina
Nationale Akademie
der Wissenschaften

Curriculum Vitae Professor Dr Laura Gagliardi

Image: University of Chicago

Name: **Laura Gagliardi**
Date of birth: **6 April 1968**

Research Priorities: Development of quantum chemical methods, catalysis, spectroscopy, photochemistry, quantum materials

Laura Gagliardi is an Italian-American chemist. She develops novel quantum chemical methods and applies them to study phenomena related to sustainable energies. Using the methods she develops, she also investigates molecular systems and materials which are relevant for catalysis, carbon separation, photochemical processes, spectroscopy, and heavy metal chemistry.

Academic and Professional Career

since 2020	Richard and Kathy Leventhal Professor, Department of Chemistry, University of Chicago, Chicago, USA
since 2020	Director, Chicago Center for Theoretical Chemistry, University of Chicago, Chicago, USA
2014 - 2020	Distinguished McKnight Professor, University of Minnesota, Minneapolis, USA
2012 - 2020	Director, Chemical Theory Center, University of Minnesota, Minneapolis, USA
2009 - 2020	Professor, University of Minnesota, Minneapolis, USA
2006 - 2008	Associate Professor, University of Geneva, Geneva, Switzerland
2000 - 2005	Assistant Professor, University of Palermo, Palermo, Italy
1998 - 1999	Postdoctoral Fellow, University of Cambridge, Cambridge, UK
1997	Ph.D. in Theoretical Chemistry, University of Bologna, Bologna, Italy

Functions in Scientific Societies and Committees

since 2022	Editor in Chief, Journal "Chemical Theory and Computation" (ACS), USA
2021	Associate Editor, Journal of the American Chemical Society (ACS), USA
2021 - 2026	Member, Board of Directors, Physical Division, ACS, USA
since 2020	Diversity Committee, Department of Chemistry, University of Chicago, Chicago, USA
since 2019	Member, Chemical Science Roundtable, Engineering and Medicine, National Academy of Sciences, USA
since 2018	Associate Editor, Journal of Catalysis, USA
2017 - 2020	Member, Board of Directors, Division of Chemical Physics, American Physical Society, USA
2016 - 2020	Associate Editor, Journal of Chemical Theory and Computation, USA
2013 - 2016	Member, Advisory Board, Physical Chemical Division, ACS, USA
2012 - 2013	Member, Board of Directors, Theoretical Chemistry Subdivision, ACS, USA
	Member, Editorial Board: since 2019 Physical Chemistry Chemical Physics, since 2015 Chemical Reviews, since 2014 ACS Central Science, 2014 - 2016 Inorganic Chemistry, 2013 - 2018 The Journal of the American Chemical Society, 2012 - 2016 Journal of Chemical Theory and Computation, 2011 - 2016 Journal of Physical Chemistry, since 2009 Theoretical Chemistry Accounts

Project Coordination, Membership in Collaborative Research Projects

2022 - 2026	Director and Principal Investigator, Catalyst Design for Decarbonization Center (CD4DC), U.S. Department of Energy, USA
2022 - 2025	Principal Investigator, Diffusion of Water Confined in Patterned Hydrophilic-Hydrophobic Nanopores, National Science Foundation (NSF), USA and German Research Foundation (DFG), Germany
2022 - 2024	Principal Investigator, Exascale Multireference Wave Function Theory Method for Polymer Upcycling Catalysis, U.S. Department of Energy, USA
2020 - 2024	Principal Investigator, Multi-Configuration Pair-Density Functional Theory for Magnetic Systems, Air Force Office of Scientific Research (AFOSR), USA
2020 - 2024	Co-Principal Investigator, GE Additively Manufactured Integrated Reservoir to Extract Water Using Adsorbents and Thermally-Enhanced Recovery (AIR2WATER), Defense Advanced Research Projects Agency (DARPA) and General Electric (GE) Company, Boston, USA

2017 - 2022 Co-Principal Investigator, Actinide Center of Excellence National Nuclear Security Administration, U.S. Department of Energy, USA

2015 - 2024 Principal Investigator, Multi-Configuration Pair-Density Functional Theory (CHE-1464536), NSF, USA

2014 - 2022 Director and Principal Investigator, Inorganometallic Catalyst Design Center, Energy Frontier Research Center (EFRC), University of Chicago, Chicago, USA – U.S. Department of Energy, USA

2012 - 2022 Principal Investigator, Nanoporous Materials Genome Center (NMGC), U.S. Department of Energy, USA

2012 - 2021 Director, Principal Investigator and Co-Principal Investigator, Predictive Hierarchical Modeling of Chemical Separations and Transformations in Functional Nanoporous Materials: Synergy of Electronic Structure Theory, Molecular Simulations, Machine Learning, and Experiments, U.S. Department of Energy, Washington USA

2010 Grant, Swiss National Science Foundation (SNF), Switzerland

2009 - 2022 Principal Investigator, Quantum Chemical Treatment of Strongly Correlated Magnetic Systems Based on Heavy Elements, U.S. Department of Energy, USA

Honours and Awarded Memberships

2023 Pauling Medal, American Chemical Society, USA

since 2022 Member, German National Academy of Sciences Leopoldina, Germany

since 2021 Member, National Academy of Sciences, USA

2021 Faraday Lectureship Prize, Royal Society of Chemistry, UK

since 2020 Member, American Academy of Arts and Sciences, USA

2020 Peter Debye Award in Physical Chemistry, The American Chemical Society, USA

since 2019 Member, International Academy of Quantum Molecular Science

2019 - 2020 McKnight Presidential Foundation Professor, University of Minnesota, Minneapolis, USA

2019 Award in Theoretical Chemistry, Physical Chemistry Division, American Chemical Society, USA

since 2018 Member, Academia Europea

2018 Humboldt Foundation Research Award, Humboldt Foundation, Bonn, Germany

since 2017 Member, World Association of Theoretical and Computational Chemists

2016 Fellow, American Physical Society (APS), USA

2016	Fellow, Royal Society of Chemistry, UK
2016	Bourke Award, Royal Society of Chemistry, UK
2016	Isaiah Shavitt Lectureship Award, Technion – Israel Institute of Technology, Haifa, Israel
2015	Visiting Professor, École Normale Supérieure de Chimie de Paris, Paris, France
2005	Visiting Scholar, Department of Chemistry, Lund University, Lund, Sweden
2003, 2005	Visiting Scholar, Department of Chemistry, University of Tokyo, Tokyo, Japan

Research Priorities

Laura Gagliardi is an Italian-American chemist. She develops novel quantum chemical methods and applies them to study phenomena related to sustainable energies. Using the methods she develops, she also investigates molecular systems and materials which are relevant for catalysis, carbon separation, photochemical processes, spectroscopy, and heavy metal chemistry.

Together with her team, Laura Gagliardi combines multi-reference theories with density functional theory. She uses classic simulations as well as progressive quantum and data science in order to discover and better understand the next generation of chemical systems and materials. These systems are practically applied in the areas of sustainability, nuclear waste disposal, and energy and water extraction.

For example, Laura Gagliardi and a team of researchers studied how water molecules from the air become trapped in metal-organic frameworks (MOFs) and how this might be a way to extract clean drinking water in the future. In certain aluminium-based MOFs, water molecules are trapped particularly well in the cavities. This is even the case with very low humidity, for example in deserts. The heat of the sun then squeezed water from the MOF.

Using x-ray crystallography and quantum chemical calculations, Laura Gagliardi was able to examine the cavities of the MOFs and analyse the underlying mechanism on the atomic level. As water molecules behave differently depending on environmental temperature and humidity, these insights can be used to help create MOFs which are optimised for certain environmental conditions. Laura Gagliardi also works on more sustainable catalysts, more efficient photovoltaics, and more reliable qubits.