



## CURRICULUM VITAE

### LAURA GAGLIARDI

#### CURRENT PROFESSIONAL ADDRESS

Department of Chemistry, University of Minnesota  
 207 Pleasant St. SE (Office 229)  
 Minneapolis, MN 55455-0431  
 Phone: (612) 625-8299  
 Email: [gagliard@umn.edu](mailto:gagliard@umn.edu)  
 Web page: <http://www.chem.umn.edu/groups/gagliardi>

#### ACADEMIC RANK

McKnight Presidential Endowed Chair, Distinguished McKnight University Professor, Professor of Chemistry, and Graduate Faculty Appointment in Chemical Engineering and Materials Science, University of Minnesota

#### EDUCATION

Degree	Institution	Degree Granted
M.A./M.S.	University of Bologna, Italy	1992
Ph.D./J.D.	University of Bologna, Italy [Ph.D. advisor: Gian Luigi Bendazzoli]	1997

#### PROFESSIONAL EXPERIENCE

##### *University of Minnesota*

McKnight Presidential Endowed Chair	2019-present
Distinguished McKnight University Professor	2014-present
Professor	2009-present
Director, Inorganometallic Catalyst Design Center EFRC	2014-present
Graduate Appointment in Chemical Engineering and Materials Science	2012-present
Director, Chemical Theory Center	2012-present
Director, Nanoporous Materials Genome Center	2012 - 2014

##### *Previous Employment*

Associate Professor, University of Geneva (Switzerland)	2005 - 2009
Assistant Professor, University of Palermo (Italy)	2000 - 2004

##### *Postdoctoral Appointments*

University of Cambridge (U.K.)	1998 - 2000
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##### *Graduate Appointments*

University of Bologna (Italy)	1993 - 1997
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## RESEARCH INTERESTS AND EXPERTISE

Development of novel quantum chemical methods for strongly correlated systems. Combination of first principle methods with classical simulation techniques. The applications are focused on the computational design of novel materials and molecular systems for energy-related challenges. Special focus is devoted to modeling catalysis and spectroscopy in molecular systems; catalysis and gas separation in porous materials; photovoltaic properties of organic and inorganic semiconductors; separation of actinides.

## SELECTED HONORS AND AWARDS

- 2020: Elected Member of the American Academy of Arts and Sciences
- 2020: Peter Debye Award in Physical Chemistry from the American Chemical Society
- 2019: Elected Member of the International Academy of Quantum Molecular Science
- 2019: McKnight Presidential Endowed Chair
- 2019: Award in Theoretical Chemistry from the Physical Chemistry Division of the American Chemical Society
- 2018: Elected Member of Academia Europea
- 2018: Humboldt Foundation Research Award
- 2017: Elected Member of the World Association of Theoretical and Computational Chemists
- 2016: Fellow of the American Physical Society
- 2016: Fellow of the Royal Society of Chemistry
- 2016: Bourke Award of the Royal Society of Chemistry
- 2016: Fellow of the Institute on the Environment, University of Minnesota
- 2016: Isaiah Shavitt lectureship award - Israel Institute of Technology
- 2014: Distinguished McKnight University Professor
- 2010: Swiss National Science Foundation Grant
- 2005: Visiting Professor Lund University, Sweden Department of Chemistry
- 2004: Annual award of the International Academy of Quantum Molecular Science to scientists under 40
- 2003: Visiting Professor University of Tokyo, Department of Chemistry

## NAMED LECTURES

- 2019, March 19: Charles Coulson Lecture, University of Georgia
- 2018, February 28: The Borden Endowed Lecture in Theoretical Chemistry, University of Washington, Seattle

## CURRENT MEMBERSHIP IN PROFESSIONAL ORGANIZATIONS

American Chemical Society, American Physical Society, American Association for the Advancement of Science, Royal Society of Chemistry; Academia Europea

## SERVICE AND PUBLIC ENGAGEMENT

### Service To The Discipline/Profession/Interdisciplinary Area(s)

#### *Editorships*

Associate Editor, *Journal of Chemical Theory and Computation* (2016-present)

Member, Editorial Advisory Board, *Physical Chemistry Chemical Physics* (2019-present); *Journal of Catalysis* (2018-present); *Chemical Reviews* (2015-present); *ACS Central Science* (2014-present); *The*

*Journal of the American Chemical Society* (2013-2018); *Inorganic Chemistry* (2014-2016); *Journal of Chemical Physics* (2010-2016); *Theoretical Chemistry Accounts* (2009-present); *Journal of Chemical Theory and Computation* (2012-2016); *Journal of Physical Chemistry* (2011-2016)

### ***Committee memberships***

Elected Officer of the American Physical Society Division of Chemical Physics (2017-2020); Elected Alternate Councilor for the Physical Chemical Division of the American Chemical Society (2013-2016); Chair of the Theoretical Chemistry Subdivision Executive Committee of the American Chemical Society (2012-2013); Officer of the Theoretical Chemistry Subdivision Executive Committee of the American Chemical Society (2011-2012); Member of the Chemical Science Roundtable of the National Academy of Sciences, Engineering and Medicine (2019-present)

### ***Organization of conferences, workshops, panels, symposia***

- 2019: 7th Annual OpenMolcas Developers' Workshop, June 2019, Minneapolis, USA
- 2019: DOE Workshop on Earth Abundant Catalysis, April 2019 Rockville, USA
- 2019: APS DCOMP Program Chair of the APS March Meeting 2019
- 2018: International Conference on Coordination Chemistry ICC2018 symposium "S28 Theoretical Coordination Chemistry", Sendai Japan
- 2018: APS March Meeting 2018 symposium 'Excited States and Non-adiabatic Dynamics in Molecular Systems', Los Angeles, USA
- 2017: The Minnesota Workshop on ab Initio Modeling in Solid State Chemistry with CRYSTAL, Minneapolis, USA
- 2016: Short course on reaction mechanisms for the Inorganometallic Catalyst Design Center University of Minnesota, Minneapolis, USA
- 2015: Crash course on catalysis for the Inorganometallic Catalyst Design Center University of Minnesota, Minneapolis, USA
- 2015: 249th ACS national meeting symposium 'Design of Materials and Chemical Processes: The Genomic Approach', Denver, USA
- 2014: 247th ACS national meeting symposium 'Heavy Element Chemistry', Dallas, USA
- 2012: Electronic Structure Theory for Strongly Correlated Systems, Palermo Italy, a conference in honor of Per-Åke Malmqvist
- 2012: 244th ACS national meeting symposium 'Bridging the gap between quantum chemistry and classical simulations', Philadelphia, USA
- 2008: Swiss Summer School in Computational Chemistry, Villars, Switzerland
- 2007: Molcas Workshop, Villars, Switzerland
- 2006: Symposium in honor of Björn Roos, Crete
- 2005: European Summer School in Quantum Chemistry, Palermo, Italy
- 2000: European Summer School in Quantum Chemistry, Riolo Terme, Italy

### ***Outreach Lectures and Activities***

- 2018: January 31, KAUST, Meeting with women graduate students, postdoctoral associates and staff to discuss about career opportunities and challenges for women in science, especially in the Middle East
- 2017: October 12, Humboldt University, Berlin, Meeting with women graduate students and postdoctoral associates to discuss about career opportunities and challenges for women in science
- 2017: June 6-August 10, Organizer of the Undergraduate Theoretical Chemistry Summer Fellowship Program at the University of Minnesota. The Chemical Theory Center hosted four undergraduate students to perform summer research in theoretical chemistry.

- 2017: May 31, Imperial College, London Meeting with women graduate students and postdoctoral associates to discuss about career opportunities and challenges for women in science
- 2017: April 4, 253rd ACS National Meeting post-doctoral breakfast in which established female professors meet young female post-docs, with the aim of sharing their experience as women in computational chemistry and in mentoring the next-generation
- 2017: February 23, Brigham Young University, Meeting with women undergraduate students and women faculty to discuss about women in science
- 2016: April 5, École Normale Supérieure Paris, “Journée des Jeunes Chercheurs: meeting with French chemistry graduate students to discuss the differences and similarities between a European and an American scientific career”
- 2015: November 20, Ripon College, WI, Invited lecture on “Women pursuing careers in science: challenges and opportunities”
- 2015: May 11, Boston University, Meeting with women undergraduate students and women faculty to discuss about women in science
- 2010: October 28, Stanford University, Distinguished Women in Science Colloquia

Since 2017: Summer Fellowship in Theoretical Chemistry; Raise money to host 5-10 undergraduates to perform summer research for 10 weeks at the Chemical Theory Center, University of Minnesota

### **Service To The University of Minnesota**

Director of the Energy Frontier Research Center Inorganometallic Catalyst Design Center, University of Minnesota, 2014-present  
 Director of the Nanoporous Materials Genome Center, University of Minnesota, 2012-2014  
 Director of the Chemical Theory Center, University of Minnesota, 2012-present  
 Planning Staffing and Resources Committee, Department of Chemistry, 2013-2016  
 (Chair in 2014-2015)  
 Graduate Student Admissions Committee, Department of Chemistry, 2012-2018  
 Graduate Student Symposium Committee, Department of Chemistry, 2011-2013  
 Faculty Search Committee, Department of Chemistry, 2010-2012; 2014; 2015; 2018-present  
 Faculty Award Committee, College of Science and Engineering, 2018-present

### **TEACHING AND CURRICULUM DEVELOPMENT**

#### **Courses**

##### *University of Minnesota*

CHEM 4021/8021, Computational Chemistry (3/4 credits)  
 CHEM 4502, Introductory Quantum Mechanics (3 credits)  
 CHEM 8552, Advanced Quantum Chemistry II: Electronic Structure Theory (4 credits)

##### *At Other Institutions*

Computational Chemistry (Masters and Doctoral)  
 Group theory in chemistry (Undergraduate)  
 Molecular Spectroscopy (Masters)  
 Statistical Thermodynamics (Graduate)

#### **Curriculum Development**

I have developed from scratch CHEM 8552, Advanced Quantum Chemistry II: Electronic Structure Theory. I have designed electronic presentation and course notes for CHEM 4502 now used by students and other instructors.

**ADVISING AND MENTORING**

Advisor to 36 postdoctoral scholars (6 current), 24 doctoral students (12 current), 9 masters students, 39 undergraduate (1 current) and 4 high-school researchers

**INVITED PRESENTATIONS**

More than 120 invited talks at national and international conferences; more than 90 invited seminars at various national and international universities, research laboratories and companies.

**PUBLICATIONS**

Author of more than 350 publications in peer-reviewed journals