

## LAURA GAGLIARDI

### PROFESSIONAL ADDRESS

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### ACADEMIC RANK

Richard and Kathy Leventhal Professor of Chemistry and Molecular Engineering University of Chicago

### EDUCATION

Degree	Institution	Date Degree Granted
M.A./M.S.	University of Bologna, Italy	1992
Ph.D.	University of Bologna, Italy	1997

### PROFESSIONAL EXPERIENCE

#### *University of Chicago*

Richard and Kathy Leventhal Professor Department of Chemistry, Pritzker School of Molecular Engineering, and James Franck Institute 2020-present

Staff Scientist, Argonne National Laboratory 2020-present

Director, Catalyst Design for Decarbonization Center EFRC 2022-present

Director of the Chicago Center for Theoretical Chemistry 2020-2023

#### *University of Minnesota, Twin Cities*

McKnight Presidential Endowed Chair 2019-2020

Distinguished McKnight University Professor 2014-2020

Professor of Chemistry 2009-2020

Director, Inorganometallic Catalyst Design Center EFRC 2014-2023

Director, Chemical Theory Center 2012-2020

Director, Nanoporous Materials Genome Center 2012-2014

#### *University of Geneva, Switzerland*

Associate Professor 2005-2009

#### *University of Palermo, Italy*

Assistant Professor 2002-2005

#### *University of Bologna, Italy*

Research Associate 2000-2001

#### *Cambridge University, United Kingdom*

Postdoctoral Research Associate 1998-1999

#### *University of Bologna, Italy*

Graduate Research Assistant 1993-1997

### SELECTER HONORS AND AWARDS

The Pauling Medal Award 2023

Fred Kavli Innovations in Chemistry Lecture 2022

Elected Member of the German National Academy of Sciences Leopoldina 2022

Elected Member of the National Academy of Sciences 2021

2021 Faraday Lectureship Prize of the Royal Society of Chemistry 2021

Elected Foreign Member of Accademia dei Lincei, Italy 2021

Elected Member of the American Academy of Arts and Sciences 2020

Peter Debye Award in Physical Chemistry from the American Chemical Society 2020

Award in Theoretical Chemistry Physical Chemistry Division of the ACS 2019

Elected Member of the International Academy of Quantum Molecular Science	2019
Elected Member of Academia Europea	2018
Humboldt Foundation Research Award	2018
Bourke Award of the Royal Society of Chemistry	2016
Elected Fellow of the American Physical Society	2016
Elected Fellow of the Royal Society of Chemistry	2016
University of Minnesota Distinguished McKnight University Professor	2014
Annual award of the International Academy of Quantum Molecular Sciences	2004

## RESEARCH INTERESTS

Development of novel quantum chemical methods for strongly correlated systems. Combination of first-principles 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, gas separations and water harvesting in porous materials; photovoltaic properties of semiconductors; actinides; quantum materials.

## SOFTWARE DEVELOPMENT

MOLCAS <http://www.molcas.org>; NWChem <http://www.nwchem-sw.org/>; pyscf <https://github.com/sunqm/pyscf>

## ADVISING AND MENTORING

Advisor to 38 postdoctoral scholars (7 current), 30 doctoral students (12 current), 10 masters students, 44 undergraduates (2 current) and 6 high-school researchers

**INVITED PRESENTATIONS AT CONFERENCES, SEMINARS, OUTREACH LECTURES:**  
more than 300

## SELECTED SERVICE AND PUBLIC ENGAGEMENT

**Editorships** Editor in Chief, *Journal of Chemical Theory and Computation* (2022-present); Associate Editor, *The Journal of American Chemical Society* (2021); Associate Editor, *Journal of Chemical Theory and Computation* (2016-2020); Member, Editorial Advisory Board, *Physical Chemistry Chemical Physics* (2019-present); *Journal of Catalysis* (2018-present); *ACS Central Science* (2014-present); *Chemical Reviews* (2015-2023);

**Committee Memberships** Elected Officer of the Physical Division of the American Chemical Society (2021-2026; Chair in 2023) 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 (2019-2022);

**Advisory Boards** Member of the Department of Energy Basic Energy Sciences Advisory Committee (<https://science.osti.gov/bes/besac/Members>) (2021-present).

## PUBLICATION LIST

(Google Scholar: <https://scholar.google.com/citations?user=7rJTBR0AAAAJ&hl=en>)