Laura Lupi

(+39) 06 57337250

laura.lupi@uniroma3.it

Tenure-Track Researcher

February 2019 - Present **Roma Tre University - Department of Mathematics and Physics**

University Assistant

August 2018 - January 2019 **University of Vienna - Department of Physics** Computational Physics Group: Prof. Christoph Dellago

Qualifications

August 2018 **Italian National Habilitation** as Associate Professor of Physics

Postdoctoral Research

September 2012 - July 2018 **University of Utah - Department of Chemistry** Advisor: Prof. Valeria Molinero

February 2012 - May 2012 **University of Perugia - Department of Physics** Advisor: Prof. Daniele Fioretto

Education

February 2012 **Ph.D. in Physics**, University of Perugia, Perugia, Italy
Advisor: Prof. Daniele Fioretto
Thesis Title: *Water at the interface with molecules of biological interest: from sugars to proteins.*

Jan-Aug 2010 **Visiting Student**, Colorado State University, Colorado, USA
Advisor: Prof. Branka Ladanyi

September 2008 **M.S. in Physics**, University of Perugia, Perugia, Italy
Advisor: Prof. Daniele Fioretto
Thesis Title: *Hydration water dynamics in water/lysozyme solutions by inelastic light scattering.*

February 2006 **B.S. in Physics**, University of Perugia, Perugia, Italy
Advisor: Prof. Daniele Fioretto
Thesis Title: *Study of the Rytov dip in liquid quinoline by depolarized light scattering.*

Research Experience

Postdoctoral Research

Department of Chemistry, University of Utah
Project I: **Mechanism of heterogeneous nucleation**
Description: I developed a coarse grained model for water-carbon systems which allowed for the first molecular dynamics simulation study of heterogeneous nucleation of ice. We showed that ordering of liquid water at the interface with soot in the atmosphere is responsible for lowering the entropy of the liquid and thus the nucleation barrier. For both

rigid and soft organic surfaces our results demonstrated that nucleation proceeds through a single step mechanism, as assumed by classical nucleation theory.

Project II: **Role of stacking disorder in ice nucleation**
Description: I used advanced sampling techniques and free energy calculations to investigate the role of stacking disorder in the pathway to homogeneous ice nucleation. We showed that nucleation through stacking disordered ice is faster than through hexagonal ice, which is the stable polymorph of bulk ice. The results published in Nature have significant implications in clouds modelling.

Project III: **Engineering of materials for technological application**
Description: I led and contributed to a variety of projects ranging from the mechanism of nucleation of mesophases from isotropic mixtures of nanoparticles, to the mechanism of molecular recognition of ice by synthetic molecules and their role in ice recrystallization inhibition, to the study of transport and water diffusion in fuel cell membranes.

Graduate Research

Dept. of Physics, University of Perugia - Dept. of Chemistry, Colorado State University
Project: **Structure and dynamics of water at the interface with biologically relevant molecules**
Description: With the combined use of broadband depolarized light scattering and classical molecular dynamics simulations, I was able to unravel for the first time the contribution to the spectrum arising from hydration water in biologically relevant conditions.

Honors & Awards

September 2016	**Best Poster Award** University of Utah Postdoc Poster Competition $500 travel grant
August 2015	**Best Poster Award** Gordon Research Conference - Chemistry and Physics of Liquids $410 travel grant & talk at GRC
September 2011	**Special Mention for Best Oral Communication** XCVII National Congress of the Italian Society of Physics Invited paper to Italian Society of Physics Journal

Publications

Peer-Reviewed Published Manuscripts, 869 citations, h-index 15

[1] Maile Marriott, **Laura Lupi**, Abhinaw Kumar, and Valeria Molinero, "Following the nucleation pathway from disordered liquid to gyroid mesophase," *The Journal of Chemical Physics*, 150, 164 902, **2019**.

[2] Yuqing Qui, **Laura Lupi**, and Valeria Molinero, "Is water at graphite surfaces ice-like or vapor-like?" *The Journal of Physical Chemistry B*, 122, 3626–3634, **2018**.

[3] **Laura Lupi**, Arpa Hudait, Baron Peters, Michael Grunwald, Ryan Gotchy Mullen, Andrew H Nguyen, and Valeria Molinero, "Role of stacking disorder in ice nucleation," *Nature*, 551, 218–222, **2017**.

[4] Pavithra M. Naullage, **Laura Lupi**, and Valeria Molinero, "Molecular recognition of ice by fully flexible molecules," *The Journal of Physical Chemistry C*, 121, 26 949–26 957, **2017**.

[5] **Laura Lupi**, Rebecca Hanscam, Yuqing Qiu, and Valeria Molinero, "Reaction coordinate for ice crystallization on a soft surface," *The Journal of Physical Chemistry Letters*, 8, 4201–4205, **2017**.

[6] **Laura Lupi**, Baron Peters, and Valeria Molinero, "Pre-ordering of interfacial water in the pathway of heterogeneous ice nucleation does not lead to a two-step crystallization mechanism," *The Journal of Chemical Physics*, 145, 211 910, **2016**.

[7] Arpa Hudait, Siwei Qiu, **Laura Lupi**, and Valeria Molinero, "Free energy contributions and structural characterization of stacking disordered ices," *Physical Chemistry Chemical Physics*, 18, 9544–9553, **2016**.

[8] Lucia Comez, Marco Paolantoni, Silvia Corezzi, **Laura Lupi**, Paola Sassi, Assunta Morresi, and Daniele Fioretto, "Aqueous solvation of amphiphilic molecules by extended depolarized light scattering: The case of trimethylamine-n-oxide," *Physical Chemistry Chemical Physics*, 18, 8881–8889, **2016**.

[9] Lucia Comez, Marco Paolantoni, **Laura Lupi**, Paola Sassi, Silvia Corezzi, Assunta Morresi, and Daniele Fioretto, "Hydrophobic hydration in water–tert-butyl alcohol solutions by extended depolarized light scattering," *The Journal of Physical Chemistry B*, 119, 9236–9243, **2015**.

[10] **Laura Lupi**, Arpa Hudait, and Valeria Molinero, "Heterogeneous nucleation of ice on carbon surfaces," *Journal of the American Chemical Society*, 136, 3156–3164, **2014**.

[11] **Laura Lupi** and Valeria Molinero, "Does hydrophilicity of carbon particles improve their ice nucleation ability?" *The Journal of Physical Chemistry A*, 118, 7330–7337, **2014**.

[12] **Laura Lupi**, Noah Kastelowitz, and Valeria Molinero, "Vapor deposition of water on graphitic surfaces: Formation of amorphous ice, bilayer ice, ice i, and liquid water," *The Journal of chemical physics*, 141, 18C508, **2014**.

[13] Lucia Comez, **Laura Lupi**, Assunta Morresi, Marco Paolantoni, Paola Sassi, and Daniele Fioretto, "More is different: Experimental results on the effect of biomolecules on the dynamics of hydration water," *The journal of physical chemistry letters*, 4, 1188–1192, **2013**.

[14] **Laura Lupi**, Lucia Comez, Marco Paolantoni, Stefania Perticaroli, Paola Sassi, Assunta Morresi, Branka M Ladanyi, and D Fioretto, "Hydration and aggregation in mono-and disaccharide aqueous solutions by gigahertz-to-terahertz light scattering and molecular dynamics simulations," *The Journal of Physical Chemistry B*, 116, 14 760–14 767, **2012**.

[15] Lucia Comez, **Laura Lupi**, Marco Paolantoni, Francesca Picchiò, and Daniele Fioretto, "Hydration properties of small hydrophobic molecules by brillouin light scattering," *The Journal of chemical physics*, 137, 114 509, **2012**.

[16] **Laura Lupi**, Lucia Comez, Marco Paolantoni, Daniele Fioretto, and Branka M Ladanyi, "Dynamics of biological water: Insights from molecular modeling of light scattering in aqueous trehalose solutions," *The Journal of Physical Chemistry B*, 116, 7499–7508, **2012**.

[17] Paola Sassi, Stefania Perticaroli, Lucia Comez, **Laura Lupi**, Marco Paolantoni, Daniele Fioretto, and Assunta Morresi, "Reversible and irreversible denaturation processes in globular proteins: From collective to molecular spectroscopic analysis," *Journal of Raman Spectroscopy*, 43, 273–279, **2012**.

[18] **Laura Lupi**, "Hydration properties of carbohydrates: A clue from molecular dynamics," *Nuovo Cimento-C*, 35, 81, **2012**.

[19] **Laura Lupi**, Lucia Comez, Claudio Masciovecchio, Assunta Morresi, Marco Paolantoni, Paola Sassi, Filippo Scarponi, and Daniele Fioretto, "Hydrophobic hydration of tert-butyl alcohol studied by brillouin light and inelastic ultraviolet scattering," *The Journal of chemical physics*, 134, 055 104, **2011**.

[20] Barbara Rossi, Lucia Comez, **Laura Lupi**, Silvia Caponi, and Flavio Rossi, "Vibrational properties of cyclodextrin–water solutions investigated by low-frequency raman scattering: Temperature and concentration effects," *Food Biophysics*, 6, 227–232, **2011**.

[21] Barbara Rossi, Lucia Comez, Daniele Fioretto, **Laura Lupi**, Silvia Caponi, and Flavio Rossi, "Hydrogen bonding dynamics of cyclodextrin–water solutions by depolarized light scattering," *Journal of Raman Spectroscopy*, 42, 1479–1483, **2011**.

[22] Stefania Perticaroli, Lucia Comez, Marco Paolantoni, Paola Sassi, **Laura Lupi**, Daniele Fioretto, Alessandro Paciaroni, and Assunta Morresi, "Broadband depolarized light scattering study of diluted protein aqueous solutions," *The Journal of Physical Chemistry B*, 114, 8262–8269, **2010**.

Book Chapters

[23] **Laura Lupi**, Lucia Comez, Marco Paolantoni, Paola Sassi, Assunta Morresi, and Daniele Fioretto, "Influence of sucrose on surrounding water by extended frequency range depolarized light scattering," in *Sucrose: Properties, Biosynthesis, and Health Implications*, Salvatore Magazù, Ed., **2013**, ch. 3.

Contributed and Invited Talks

[1] **Laura Lupi**, and Valeria Molinero, "Mechanisms of ice nucleation and ice growth inhibition", Conference on Frontiers in Water Biophysics (FWB) - Erice (Italy) September **2019**

[2] **Laura Lupi**, "Mechanisms of homogeneous and heterogeneous ice nucleation", Invited talk - University of Vienna, Faculty of Physics, Aerosol and Environmental Physics Group - Vienna (Austria) January **2019**

[3] **Laura Lupi**, Arpa Hudait, Rebecca Hanscam, Yuqing Qiu, and Valeria Molinero, "How the presence of foreign surfaces impact the rates of ice nucleation?", "Atmospheric Surface Science" session of the European Geosciences Union (EGU) General Assembly, Vienna (Austria) April **2018**

[4] **Laura Lupi** and Valeria Molinero, "Role of stacking disorder on the barrier and pathway of ice nucleation", Invited talk - University of Trieste – Trieste (Italy) April **2018**

[5] **Laura Lupi** and Valeria Molinero, "Unravelling the mechanisms of homogeneous and heterogeneous nucleation of ice", Invited talk - University of North Carolina – Chapel Hill (NC) December **2017**

[6] **Laura Lupi**, Arpa Hudait, Baron Peters, Michael Grünwald, Rebecca Hanscam, Yuqing Qiu, and Valeria Molinero, "Is classical nucleation theory valid for ice nucleation?", 253rd ACS National Meeting, San Francisco (CA) April **2017**

[7] **Laura Lupi**, Baron Peters and Valeria Molinero, "Role of stacking disorder in ice nucleation", Towards a Molecular Level Understanding of Atmospheric Aerosols, Santa Cruz (CA) August **2016**

[8] **Laura Lupi**, Arpa Hudait, Baron Peters and Valeria Molinero, "Nucleation of ice at hydrophobic and hydrophilic interfaces", KAUST International Conference on Physics and Chemistries at Hydrophobic Interfaces - KAUST (Saudi Arabia) February **2016**

[9] **Laura Lupi**, Arpa Hudait, Baron Peters and Valeria Molinero, "Mechanism of homogeneous and heterogeneous nucleation of ice", Invited talk - University of Texas A&M – College Station (TX) October **2015**

[10] **Laura Lupi**, Arpa Hudait, Baron Peters and Valeria Molinero, "Rate limiting step for the nucleation of ice", 3rd Conference on Frontiers in Water Biophysics (FWB) - Erice (Italy) September **2015**

[11] **Laura Lupi**, Arpa Hudait, Baron Peters and Valeria Molinero, "Rate limiting step for the nucleation of ice", Gordon Research Conference (GRC) Chemistry and Physics of Liquids – BEST POSTER PRICE - Holderness (NH) August **2015**

[12] **Laura Lupi**, Arpa Hudait, Baron Peters and Valeria Molinero, "Rate limiting step for the nucleation of ice", Gordon Research Seminars (GRS) Chemistry and Physics of Liquids - Holderness (NH) August **2015**

[13] **Laura Lupi**, Arpa Hudait and Valeria Molinero, "Heterogeneous nucleation of ice on carbon surfaces", 13th International Conference on Physics and Chemistry of ice - Hanover (NH) March **2014**

[14] **Laura Lupi**, Lucia Comez, Marco Paolantoni, Daniele Fioretto and Branka M. Ladanyi, "Hydration water of biological molecules: depolarized light scattering and molecular dynamics simulations", XCVII National Meeting, Italian Society of Physics - L'Aquila (Italy) September **2011**

[15] **Laura Lupi**, Lucia Comez, Branka M. Ladanyi, Marco Paolantoni and Daniele Fioretto, "Influence of carbohydrates on surrounding water molecules", Workshop on Soft Matter - Parma (Italy) February **2011**

Poster Presentations

[1] **Laura Lupi**, Arpa Hudait, Baron Peters and Valeria Molinero, "Role of stacking disorder in nucleation, growth and stability of ice", Postdoc Appreciation Day University of Utah - BEST POSTER AWARD - Salt Lake City (UT) September **2016**

[2] **Laura Lupi**, Arpa Hudait, Baron Peters and Valeria Molinero, "Role of stacking disorder in nucleation, growth and stability of ice", CAICE Annual Meeting - San Diego (CA) April **2016**

[3] **Laura Lupi**, Valeria Molinero, "Rate limiting step for the nucleation of ice", GRC - BEST POSTER AWARD - Holderness (NH) August **2015**

[4] **Laura Lupi**, Arpa Hudait and Valeria Molinero, "Heterogeneous nucleation of ice on carbon surfaces", ACTC - Telluride (CO) July **2014**

[5] **Laura Lupi** and Valeria Molinero, "Does hydrophilicity of carbon particles improve their ice nucleation ability?", GRC Chemistry and physics of liquids - Holderness (NH) August **2013**

[6] **Laura Lupi** and Valeria Molinero, "Does hydrophilicity of carbon particles improve their ice nucleation ability?", Mini stat mech meeting - Berkeley (CA) January **2013**

[7] **Laura Lupi**, Lucia Comez, Daniele Fioretto, Marco Paolantoni and Branka M. Ladanyi, "Water dynamics in sugar aqueous solutions: Molecular dynamics simulations and depolarized light scattering experiments", EMLG/JMLG - Warsaw (Poland) September **2011**

Teaching Experience, Mentoring and Science Outreach

Teaching experience

- Professor of the Atomic and Molecular Physics class, University of Roma Tre (Spring 2020)
- Teaching Assistant for the Condensed Matter Physics class, University Roma Tre (Fall 2019)
- Professor of the Computational Physics I class, University of Vienna (Fall 2018)
- Teaching Assistant for the Molecular dynamics simulations class, University of Utah (Spring 2016)
- Teaching Assistant for Electromagnetism, University of Perugia (Fall 2009)
- Volunteer Teacher at Center for middle and high school students "PortoFranco", Perugia, Italy (2008-2012)

Student mentoring

- During my PhD I mentored a master student (Francesca Picchiò). As a postdoc I mentored four undergraduate students for summer research internships (Michael Goytia – Summer 2015, Rebecca C. Hanscam – Summer 2016, Maile M. Marriott and Samantha Walker - Summer 2017) and two graduate students (Pavitra Naullage and Maryam Ghiassee).

Scientific outreach

- I co-developed the workshop "Growth of crystals in 3D" and presented to high school students during the Science Day events organized by the University of Utah.
- I contributed to the exhibit "Water" exposed in the contemporary museum of science and art The Leonardo in Salt Lake City.
- I led experiments of general physics for high school students within the project "Progetto Lauree Scientifiche" (Project Scientific Degrees), organized by the University of Perugia in collaboration with local High Schools.

Professional services

Reviewer for International Journals:

- Physical Review Letters - ACS nano - Nanoscale - Communications Physics - Journal of Chemical Physics - Journal of Physical Chemistry - Atmospheric Chemistry and Physics - Canadian Geotechnical Journal

Organization of International Conferences:

- Member of the organizing committee of the Congress on Water Under Extreme Conditions 2019.
- Co-Convener and chair of the "Atmospheric Surface Science" session of the European Geosciences Union (EGU) General Assembly 2018.
- Member of the organizing committee of the Conference on Frontiers in Water Biophysics 2012.

Service as committee member:

- Member of the committee for selection of one candidate for a research position at the Department of Physics of Roma Tre University, Fall 2019.
- Member of the committee for Theses defence at the Department of Physics of Roma Tre University, Fall 2019.