



TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO

ID CODE 4326

I the undersigned asks to participate in the public selection, for qualifications and examinations, for the awarding of one type B fellowships at Dipartimento di Fisica, Scientist- in - charge **Prof. Nicola Manini**

Melisa Mariel Gianetti

CURRICULUM VITAE

PERSONAL INFORMATION

Surname	Gianetti
Name	Melisa Mariel
Date of birth	21, March, 1986

PRESENT OCCUPATION

Appointment	Structure
Postdoctoral Fellow	Institute of Materials Science and Technology (INTEMA) National Council of Scientific and Technical Research (CONICET)

EDUCATION AND TRAINING

Degree	Course of studies	University	year of achievement of the degree
Degree	Chemistry	National University of Mar del Plata	2010
Specialization			
PhD	Inorganic Chemistry, Analytical Chemistry and Physical Chemistry	University of Buenos Aires	2017
Master			
Degree of medical specialization			
Degree of European specialization			
Other			

REGISTRATION IN PROFESSIONAL ASSOCIATIONS

Date of registration	Association	City



--	--	--

FOREIGN LANGUAGES

Languages	level of knowledge
Spanish	Mother tongue
English	High
German	Basic

AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2012	Ph. D. start fellowship. 3-year fellowship for graduate students to start their Ph. D. Advisors: Dr. M. Paula Longinotti and Prof. Dr. Pablo G. Debenedetti. Institute of Physics and Chemistry of Materials, Environment and Energy (INQUIMAE) and University of Buenos Aires. Organism: National Agency of Scientific and Technological Promotion (ANPCYT).
2015	Ph. D. culmination fellowship. 2-year fellowship for graduate students to finish their Ph. D. Advisors: Dr. M. Paula Longinotti and Prof. Dr. Pablo G. Debenedetti. Institute of Physics and Chemistry of Materials, Environment and Energy (INQUIMAE) and University of Buenos Aires. Organism: CONICET
2017	Postdoctoral fellowship. Advisor: Prof. Dr. Ezequiel R. Soulé. INTEMA and University of Mar del Plata. Organism: CONICET

TRAINING OR RESEARCH ACTIVITY

description of activity

During my PhD I worked on the kinetics of nucleation and crystallization of water using two different approaches. On one hand, a computer simulation approach was used. The vast varieties of existent water models make different predictions regarding thermodynamic and kinetic properties of water. Thus, it is of fundamental importance to know how the different parameters of a given model affect the predicted properties in the studied systems. For instance, in the case of water crystallization, nucleation and the existence of a liquid-liquid transition are relevant processes which are needed to be understood in detail. My particular work (*Phys. Chem. Chem. Phys.*, 18, 2016, 4102) consisted in the analysis of how the tetrahedral parameter, λ , of the monatomic water model (mW) (*J. Chem. Phys. B*, 113, 2009, 4008) influences the nucleation kinetics. It was found that when λ varies between 21 and 24, for a constant supercooling of $T/T_m = 0.845$, (λ for mW is 23.15, that is the reason for choosing 21 to 24 for the study) the nucleation rate increases 48 orders of magnitude. We could find an explanation for this observation through the Classical Nucleation Theory (CNT) related to the increase of the thermodynamic driving force, $\Delta\mu$. We also calculated the nucleation rate in free-standing thin films of supercooled liquids to study the influence of the liquid-vapor interface. It was shown that the effect of the interface in the nucleation kinetics depends on λ , being the nucleation rate higher in thin films than in bulk for $\lambda = 21$, while the opposite behavior was observed for $\lambda \geq 22$.

The other approach used for studying ice crystallization was an experimental one; we analyzed the ice crystallization rate using Atomic Force Microscopy (AFM). In our group we developed an environmental chamber to measure the thickness of the quasi-liquid layer (QLL) formed on ice surfaces below the melting temperature (*Atmos. Chem. Phys.*, 18, 2018, 14965). Relative humidity and temperature conditions were strictly controlled close to the sample. This work showed, for the first time, that if the experimental conditions are accurately controlled, the QLL thicknesses obtained by AFM lie over the lower bound of the highly disperse results reported in the literature. This allowed us to estimate upper boundaries for the QLL thicknesses, which are relevant to validate QLL theories and improve multiphase atmospheric chemistry models.



This work was extended in my PhD thesis through studying ice growth rates on a flat mica surface with AFM and the same environmental chamber (*Atmos. Chem. Phys.*, 18, 2018, 14965). We were able to measure ice growth rates for different supercooling degrees close to the melting temperature and calculate the corresponding ice growth rates (submitted to Review of Scientific Instruments). This setup has advantages with respect to previous reported techniques since temperature and relative humidity can be controlled very close to the sample, minimizing systematic errors. The most relevant result of this work is that this technique can provide kinetic information for ice growth controlling temperature and relative humidity close to the ice nucleation centers. It is a novel application which can give place to future measurements on different surfaces to study the influence of the surface in the ice growth rate.

My postdoctoral work includes the study of phase transitions in polymeric systems with molecular dynamics. One of the studied systems is a glass former supercooled polymer. We studied the relationship between its structure and its dynamic behavior through Pearson coefficients in an isoconfigurational ensemble (ICE) (*J. Chem. Phys.*, 149, 2018, 094506 and *J. Chem. Phys.*, 150, 2019, 234508). The presented method complements traditional studies of glass forming liquids in terms of mobility.

We are also studying nucleation and growth of Ag nanoparticles in presence of polyvinylpyrrolidone (PVP). Even though it is well known that PVP, as well as all structure-directing agents (SDA), have a fundamental role in shape-selective synthesis of nanoparticles, the microscopic mechanism is not completely understood. We study this system to complement experimental observations and also to contribute in modeling of nanocrystals growth and metallic nanoparticles structuring.

The formation of nanostructures of copolymers is also interesting from the modeling point of view since they can be simulated with simple models (*J. Chem. Phys. Lett.*, 8, 2017, 5053 and *J. Phys. Chem. B*, 122, 2018, 4758). Characterization of phase transition and modeling is our objects of study in these systems. This will help us to understand the microscopic processes of the formation of nanostructures and their relation with magnetic, electronic and optical properties of the resulting nanoparticles.

CONGRESSES AND SEMINARS

Date	Title	Place
Jul, 2019	-Ice growth kinetics and quasi-liquid layer thickness as revealed by environmental AFM -An alternative approach to study the heterogeneous dynamics and its consequent dynamic correlation length that emerges in a glass-former	3rd Workshop on Structure and Dynamics of Glassy, Supercooled and Nanoconfined Fluids. Buenos Aires, Argentina
Nov, 2018	-Characterization of the nucleation process of Ag nanocrystals containing Polyvinylpyrrolidone and Ethylene glycol -The dynamic and structural behavior of monomer in supercooled polymer system: a molecular dynamics study	XVI Polymers Latin American Symposium - XIV Polymers Ibero-American Congress. Mar del Plata, Argentina
May, 2018	In silico study on the anisotropic structures generation from spherical particles interacting through a non directional potential	XVIII Meeting of Surfaces and Nanostructured Materials (NANO 2018)
May, 2018	Looking at the dynamical length scales in a supercooled polymer system	XVI TREFEMAC - Regional Congress of Statistical Physics and Condensed Matter. Mar del Plata, Argentina
May, 2017	-Heterogeneous nucleation of tetrahedral liquids	XX Argentinian Congress of Physical Chemistry and Inorganic Chemistry 2017 (CAFQI 2017). Villa Carlos Paz, Argentina



	-Ice growth rate on mica with AFM	
May, 2016	Nucleation and crystallization studies of tetrahedral liquids. Effect of the liquid-vapor interface in nucleation kinetics	XVI Meeting of Surfaces and Nanostructured Materials (NANO 2016)
Apr, 2015	Homogeneous nucleation study of tetrahedral liquids in bulk and thin films	XIX Argentinian Congress of Physical Chemistry and Inorganic Chemistry 2015 (CAFQI 2015)

PUBLICATIONS

Articles in reviews
Static and dynamic correlation lengths in supercooled polymers. J. Chem. Phys. 150, 234508 (2019)
The Quasi-Liquid Layer of ice revisited: the role of temperature gradients and tip chemistry in AFM experiments. Atmos. Chem. Phys., 18, 14965-14978 (2018)
Looking at the dynamical heterogeneity in supercooled polymer system through Isoconfigurational ensemble. J. Chem. Phys. 149, 094506 (2018)
Computational investigation of structure, dynamics and nucleation kinetics of a family of modified Stillinger-Weber model fluids in bulk and free-standing thin films. Phys. Chem. Chem. Phys., 18, 4102-4111 (2016)

OTHER INFORMATION

January, 2014-March, 2014. Internship at the School of Engineering and Applied Science, Princeton University. New Jersey, USA. Pablo Debenedetti's group. Calculations of homogeneous nucleation rates for the doctoral research
August, 2012-November 2012. Internship at the School of Engineering and Applied Science, Princeton University. New Jersey, USA. Pablo Debenedetti's group. Work with postdoctoral student Amir Haji-Akbari (at present Assistant Professor of Chemical & Environmental Engineering at Yale University). Learning of advanced simulation techniques for the doctoral research.

Declarations given in the present curriculum must be considered released according to art. 46 and 47 of DPR n. 445/2000.

The present curriculum does not contain confidential and legal information according to art. 4, paragraph 1, points d) and e) of D.Lgs. 30.06.2003 n. 196.

Place and date: Mar del Plata, 5/3/2019

SIGNATURE

Melisa Mariel GIANETTI

Ph. D. in Chemistry

Updated CV, September 1st, 2019

RESEARCH INTERESTS

Structure, dynamics and transport in condensed matter and phase transitions in aqueous and polymeric systems. Nucleation and growth in condensed systems.

CURRENT POSITION

APRIL 2017 – PRESENT

Postdoctoral fellow

Nanostructured polymers group. Advisor: Prof. Dr. Ezequiel R. Soulé
Institute of Materials Science and Technology (INTEMA)
National Council of Scientific and Technical Research (CONICET)
National University of Mar del Plata, Argentina

EDUCATION

MARCH 2017

Ph. D. in Chemistry

Department of Inorganic, Analytical and Physical Chemistry. University of Buenos Aires, Argentina
Thesis: "Nucleation and crystallization kinetics of tetrahedral liquids"
Advisors: Dr. María Paula Longinotti and Prof. Dr. Pablo Gastón Debenedetti

FEBRUARY 2010

Licenciada (5-year degree, roughly equivalent to M.S.) in Chemistry

Faculty of Exact and Natural Sciences, National University of Mar del Plata, Argentina

PUBLICATION LIST

Peer Reviewed Journal Publications

- C. Balbuena, **M. M. Gianetti** and E. R. Soulé. "Static and dynamic correlation lengths in supercooled polymers." *J. Chem. Phys.* **150**, 234508 (2019).
- J. Gelman Constantín, **M. M. Gianetti**, M. P. Longinotti, and H. R. Corti. "The Quasi-Liquid Layer of ice revisited: the role of temperature gradients and tip chemistry in AFM experiments". *Atmos. Chem. Phys.*, **18**, 14965-14978 (2018)
- C. Balbuena, **M. M. Gianetti** and E. R. Soulé. "Looking at the dynamical heterogeneity in supercooled polymer system through Isoconfigurational ensemble." *J. Chem. Phys.* **149**, 094506 (2018).
- **M. M. Gianetti**, A. Haji-Akbari, M. P. Longinotti and P. G. Debenedetti. "Computational investigation of structure, dynamics and nucleation kinetics of a family of modified Stillinger-Weber model fluids in bulk and free-standing thin films." *Phys. Chem. Chem. Phys.*, **18**, 4102-4111 (2016)

INTERNSHIPS

- 01/14 – 03/14 | **School of Engineering and Applied Science, Princeton University.** New Jersey, USA.
Pablo Debenedetti's group. Calculations of homogeneous nucleation rates for the doctoral research
- 08/12 – 11/12 | **School of Engineering and Applied Science, Princeton University.** New Jersey, USA.
Pablo Debenedetti's group. Work with postdoctoral student Amir Haji-Akbari (at present Assistant Professor of Chemical & Environmental Engineering at Yale University). Learning of advanced simulation techniques for the doctoral research

FELLOWSHIPS

- 04/17 – 03/19 | **Postdoctoral fellowship.** Advisor: Prof. Dr. Ezequiel R. Soulé. INTEMA, University of Mar del Plata.
Organism: CONICET
- 04/15 – 03/17 | **Ph. D. culmination fellowship.** Advisors: Dr. M. Paula Longinotti and Prof. Dr. Pablo G. Debenedetti. Institute of Physics and Chemistry en Materials, Environment and Energy (INQUIMAE), University of Buenos Aires.
Organism: CONICET
- 02/12 – 03/15 | **Ph. D. start fellowship.** Advisors: Dr. M. Paula Longinotti and Prof. Dr. Pablo G. Debenedetti. INQUIMAE, University of Buenos Aires.
Organism: National Agency of Scientific and Technological Promotion (ANPCYT)

RELEVANT COURSES (NOT INCLUDED IN THE PH. D.)

- 2017 | **Computational Material Science**
Prof. Alejandro Rey and Oscar Matus Rivas. McGill University - UNMDP. Mar del Plata, Argentina. Qualification: 10/10
- 2014 | **Computational Tools for Scientists**
Prof. Manuel Carlevaro and Luis Pugnaroni. IFLYSIB - UNLP. La Plata, Argentina. Assistant
- 2014 | **Introduction to Disordered Systems Physics**
Prof. Tomás Grigera. INIFTA - UNLP. La Plata, Argentina. Assistant



RELEVANT CONFERENCE PRESENTATIONS (LAST 5 YEARS)

- JUL 2019 | *"Ice growth kinetics and quasi-liquid layer thickness as revealed by environmental AFM"*. **M. M. Gianetti**, J. Gelman Constantin, H. R. Corti, P. G. Debenedetti and M. P. Longinotti.
Oral presentation. 3rd Workshop on "Structure and Dynamics of Glassy, Supercooled and Nanoconfined Fluids". Buenos Aires, Argentina
- JUL 2019 | *"An alternative approach to study the heterogeneous dynamics and its consequent dynamic correlation length that emerges in a glass-former"*. C. Balbuena, **M. M. Gianetti** and E. R. Soulé.
Poster. 3rd Workshop on "Structure and Dynamics of Glassy, Supercooled and Nanoconfined Fluids". Buenos Aires, Argentina
- NOV 2018 | *"Characterization of the nucleation process of Ag nanocrystals containing Polyvinylpyrrolidone and Ethylene glycol"*. **M. M. Gianetti**, C. Balbuena and E. R. Soulé.
Poster. XVI Polymers Latin American Symposium - XIV Polymers Ibero-American Congress. Mar del Plata, Argentina
- NOV 2018 | *"The dynamic and structural behavior of monomer in supercooled polymer system: a molecular dynamics study"*. C. Balbuena, **M. M. Gianetti** and E. R. Soulé.
Poster. XVI Polymers Latin American Symposium - XIV Polymers Ibero-American Congress. Mar del Plata, Argentina
- MAY 2018 | *"In silico study on the anisotropic structures generation from spherical particles interacting through a non directional potential"*. **M. M. Gianetti**, C. Balbuena and E. R. Soulé.
Poster. XVIII Meeting of Surfaces and Nanostructured Materials (NANO 2018). Y-TEC - Berisso, Argentina
- MAY 2018 | *"Looking at the dynamical length scales in a supercooled polymer system"*. **M. M. Gianetti**, C. Balbuena and E. R. Soulé.
Poster. XVI TREFEMAC – Regional Congress of Statistical Physics and Condensed Matter. Mar del Plata, Argentina
- MAY 2017 | *"Heterogeneous nucleation of tetrahedral liquids"*. **M. M. Gianetti**, A. Haji-Akbari, M. P. Longinotti and P. G. Debenedetti
Poster. XX Argentinian Congress of Physical Chemistry and Inorganic Chemistry 2017 (CAFQI 2017). Villa Carlos Paz, Argentina
- MAY 2016 | *"Nucleation and crystallization studies of tetrahedral liquids. Effect of the liquid-vapor interface in nucleation kinetics"*. **M. M. Gianetti**, A. Haji-Akbari, M. P. Longinotti and P. G. Debenedetti
Poster. XVI Meeting of Surfaces and Nanostructured Materials (NANO 2016). Buenos Aires, Argentina
- APRIL 2015 | *"Homogeneous nucleation study of tetrahedral liquids in bulk and thin films"*. **M. M. Gianetti**, A. Haji-Akbari, M. P. Longinotti and P. G. Debenedetti
Oral presentation. XIX Argentinian Congress of Physical Chemistry and Inorganic Chemistry 2015 (CAFQI 2015). Buenos Aires, Argentina



COMPUTER SKILLS

Programming languages Python, Bash, Fortran90, \LaTeX
Simulation packages LAMMPS
OS Linux (Ubuntu), Windows
Misc XMGrace, Origin, SigmaPlot, Mendeley, Microsoft Office, NanoScope

TEACHING EXPERIENCE

04/19 – PRESENT | **Teaching Associate.** Engineering Faculty - Subject: Analytic Chemistry
FASTA University

03/18 – PRESENT | **Teaching Associate.** Department of Chemistry - Subject: Analytic
Chemistry
University of Mar del Plata (UNMDP)

04/12 – 03/17 | **Teaching Associate.** Basic common cycle (CBC) - Subject: Chemistry.
University of Buenos Aires (UBA)

04/06 – 04/08 | **Teaching Associate (as Undergraduate Student).** Department of Chem-
istry - Subject: Analytic Chemistry.
University of Mar del Plata (UNMDP)

LANGUAGES

SPANISH: Mothertongue
ENGLISH: Fluent speaking and writing. First Certificate Exam (2001)
GERMAN: Basic knowledge

REFERENCES

- Prof. Dr. Horacio R. Corti. *CNEA - CONICET*. hrcorti@tandar.cnea.gov.ar
- Prof. Dr. Pablo G. Debenedetti. *CBE - Princeton University*. pdebene@princeton.edu
- Dr. M. Paula Longinotti. *INQUIMAE - UBA*. longinot@qi.fcen.uba.ar
- Prof. Dr. Ezequiel R. Soulé. *INTEMA - CONICET - UNMDP*. ersoule@fi.mdp.edu.ar

CONTACT INFORMATION

ADDRESS: Av. Juan B. Justo 4302 - Office 238, (7600) Mar del Plata, Buenos Aires, Argentina
PHONE: +54 223 481 6600 - int: 238
CELL PHONE: +54 9 223 528 9057
EMAIL: mgianetti@fi.mdp.edu.ar - melisamariel@gmail.com

