

Felipe JIMÉNEZ ÁNGELES

CONTACT INFORMATION

Reservoir Engineering Research Institute (RERI)
ADDRESS: 595 Lytton Ave., Palo Alto, California 94301
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RESEARCH FOCUS AT RERI

1. Hydrate nucleation and growth
2. Interfacial phenomena of hydrates
3. Molecular mechanisms of hydrate antiagglomeration and inhibition
4. Interaction of liquid hydrocarbons/aqueous solutions/mineral substrates

RESEARCH SKILLS

In-depth knowledge of

- Soft Matter, Statistical Physics, Thermodynamics, Chemical Physics, Physical Chemistry, Colloids and Interface Science, and Theory of Liquids
- Molecular simulation methods (Molecular Dynamics and Monte Carlo)
- Numerical solution of non-linear differential equations from mean field theories (Poisson-Boltzmann equation) and non-linear integral equations from liquids theories
- Finite element techniques
- Programming with Fortran, C++, Mathematica, and Maple
- Simulation packages, such as ESPResSo (Extensible Simulation Package for Research on Soft matter, <http://espressomd.org/>), GROMACS (Groningen Machine for Chemical Simulations, <http://www.gromacs.org>), and Materials Studio from ACCELRYs (<http://accelrys.com/products/materials-studio/>).

Excellent scientific communication and writing skills. Ability for preparing clear and succinct manuscripts.

EDUCATION

- SEPT. 1998- Philosophy Doctor in PHYSICS
OCT. 2002 Department of Physics, UNIVERSIDAD AUTÓNOMA METROPOLITANA, Campus Iztapalapa
Thesis: "Entropic Effects and Long Range Correlations in Complex Charged Fluids"
Advisor: Prof. Marcelo LOZADA
Defense: October 3rd 2002
- SEPT. 1996- Master of Science: PHYSICS
JUNE 1998 Department of Physics, UNIVERSIDAD AUTÓNOMA METROPOLITANA, Campus Iztapalapa
Thesis: "Simple Model for a Semipermeable Membrane"
Advisor: Prof. Marcelo LOZADA
Defense: June 25th 1998
- SEPT. 1991- Bachelor of Science: PHYSICS
MAY 1996 Department of Physics, UNIVERSIDAD AUTÓNOMA METROPOLITANA, Campus Iztapalapa

WORK EXPERIENCE

- JULY 2013- | Research Scientist at RESERVOIR ENGINEERING RESEARCH INSTITUTE (RERI),
PRESENT | Palo Alto, CA
Collaborating with Prof. Abbas Firoozabadi on molecular simulation of hydrate nucleation; interfacial properties of hydrates; antiagglomeration of hydrates; wettability of hydrocarbons/brine setups on mineral substrates.
- JUNE 2012- | Visiting Scientist at INSTITUT DE CHIMIE, DE PHYSIQUE ET DES MATÉRIAUX,
JULY 2012 | UNIVERSITÉ DE LORRAINE, Metz France
Collaborating with Prof. René Messina on modeling macroion adsorption from solutions on charged surfaces using statistical mechanics theories and molecular simulations.

JUNE 2006-
JULY 2013

Research Scientist at INSTITUTO MEXICANO DEL PETRÓLEO (IMP),
México City, Mexico

Collaborating in the groups of Molecular Engineering and Flow Assurance in the following projects:

HYDRAULIC FRACTURING USING SMART MATERIALS. Contribution: Development of a code for simulating flow of hydrocarbons in fractured reservoirs.

STUDY OF BIOMOLECULES TO MODIFY THE RHEOLOGICAL PROPERTIES OF HEAVY OILS: PRODUCTION AND CHARACTERIZATION. Contribution: Molecular modeling of surfactant molecules.

BIOMOLECULES FOR ENHANCE HYDROCARBON RECOVERY IN COMPLEX RESERVOIRS. Contribution: Molecular modeling of adsorption of macromolecules on different substrates.

GAS SWEETENING BY MEANS OF SEMIPERMEABLE MEMBRANES. Contribution: Prediction of the selectivity and diffusion coefficients of the components of natural gas in different membranes using molecular dynamics simulations.

DESIGN OF POLYMERIC MEMBRANES FOR GAS SEPARATION. Contribution: Molecular modeling of the adsorption and diffusion of gases in polymeric membranes using statistical mechanics theories and molecular simulations.

DESIGN AND DEVELOPMENT OF CHEMICALS TO MODIFY THE OIL-ROCK WETTABILITY TO INCREASE OIL RECOVERY. Contribution: Molecular modeling of adsorption of oil emulsions and macromolecules on the rock surfaces and pores using statistical mechanics theories and molecular simulations.

NEW CATALYSTS OF LOW METALLIC CHARGE FOR HYDRODESULFURIZATION. Contribution: Molecular modeling of surface properties of nanomaterials using statistical mechanics theories and molecular simulations.

COLLABORATION IN THE GRADUATE STUDENT PROGRAM OF IMP. Contribution: Supervision of PhD. students, courses, seminars, and short lectures.

NOV. 2002 -
MAY 2006

Postdoctoral position at INSTITUTO MEXICANO DEL PETRÓLEO (IMP),
México City, Mexico

MOLECULAR ENGINEERING OF NANOCATALYST AND NANOTUBES. Contribution: Molecular modeling of the adsorption of molecules on nanomaterials using statistical mechanics theories and molecular simulations.

PHYSICS OF CONFINED FLUIDS. Contribution: Development of complex fluids models confined between pores and walls using statistical mechanics theories and molecular simulations.

MAY 1998-
JULY 2002

Associate Professor (Lecturer) at UNIVERSIDAD AUTÓNOMA METROPOLITANA,
Campus Iztapalapa, México City, Mexico

PHYSICS DEPARTMENT. Contribution: Undergraduate courses on calculus, differential equations, kinematics and mechanics, waves and rotations, electrostatics.

JULY 1996-
MAY 1998

Teaching assistant at UNIVERSIDAD AUTÓNOMA METROPOLITANA,
Campus Iztapalapa, México City, Mexico

PHYSICS DEPARTMENT. Contribution: Problem solutions classes, exercises revision, and exams revision, in undergraduate courses (kinematics and mechanics, waves and rotations, electrostatics).

PUBLICATIONS

1. Jiménez-Ángeles F., Firoozabadi A.; Enhanced Hydrate Nucleation Near the Limit of Stability; Submitted (2015)
2. Jiménez-Ángeles F., Firoozabadi A.; Induced Charge Density and Thin Liquid Film at Hydrate/Methane Gas Interfaces; *J. Phys. Chem. C*, **118**, 26041–26048, (2014)
3. del Río J. M., Santillan R., Vallejo I., Grolier J. P. E., Jiménez-Ángeles F., Corea M. A.; Thermodynamic Method to Study the Interaction Between NaOH and Highly Carboxylated Polymeric Particles in Solution; *J. Sol. Chem.*, **43**, 1-24 (2014)
4. Jiménez-Ángeles F., Firoozabadi A.; Nucleation of Methane Hydrates at Moderate Subcooling by Molecular Dynamics Simulations; *J. Phys. Chem. C*, **118**, 11310-11318, (2014)
5. Sanchez-Arellano E., Jiménez-Ángeles F.; Electrokinetic Properties of a Restricted Primitive Model Electrolyte in Slit-Like Nanopores: Effects of Ionic Excluded Volume; *Mol. Liq.*, **185**, 76-82, (2013)
6. Jiménez-Ángeles F.; Effects of Mixed Discrete Surface Charges on the Electrical Double Layer; *Phys. Rev. E*, Vol. **86**, 021601, (2012)
7. Jiménez-Ángeles F., Odriozola G, Lozada-Cassou M.; Entropy Effects in Self-Assembling Mechanisms: Also a View From the Information Theory; *J. Mol. Liq.*, **164**, 74-86, (2011)
8. Manzanilla-Granados H. M., Jiménez-Ángeles F., Lozada-Cassou M.; Polarity Inversion of ζ -Potential in Concentrated Colloidal Dispersions; *J. Phys. Chem. B*, **115**, 12094–12097, (2011)
9. Manzanilla-Granados H. M., Jiménez-Ángeles F., Lozada-Cassou M.; The ζ -Potential for a Concentrated Colloidal Dispersion: The Colloidal Primitive Model vs. the Cell Model; *Colloids and Surfaces A: Physicochem. Eng. Aspects* **376**, 59–66, (2011).
10. Odriozola G., Jiménez-Ángeles F., Orea P.; Assisted Crystal Growing by Tempering Metastable Vapor-Liquid Fluids; *Chem. Phys. Lett.* **501**, 466-469 (2011)
11. Jiménez-Ángeles F., Odriozola G, Lozada-Cassou M.; Stability Mechanisms for Plate-Like Nanoparticles Immersed in a Macroion Dispersion, *J. Phys.:Cond.-Matter*, Vol. 21, 424107 (2009)
12. Sánchez-Arellano E., Olivares W., Lozada-Cassou M., Jiménez-Ángeles F.; Electrokinetic Properties of Monovalent Electrolyte Confined in Charged Nanopores: Effect of Geometry and Ionic Short Range Correlations; *J. Colloids and Int. Sci.* **330**, 474–482 (2009)
13. Jiménez-Ángeles F., Doua Y., Odriozola G., Lozada-Cassou M.; Population Inversion of a Non-Additive Hard-Sphere Fluid Confined by a Cylindrical Pore. *The Journal of Physical Chemistry C*, vol. 112, 18028 (2008)
14. Gerardo Odriozola, Jiménez-Ángeles F., Lozada-Cassou M.; Entropy Driven Key-Lock Assembly, *J. Chem. Phys.* **129**, 111101 (2008)
15. Jiménez-Ángeles F. and Lozada-Cassou M.; On the Regimes of Charge Reversal, *J. Chem. Phys.*, **128**, 174701 (2008)
16. Aguilar G. E., Jiménez-Ángeles F., Yu J., Lozada-Cassou M.; Van der Waals-Like Isotherms in a Confined Electrolyte by Spherical and Cylindrical Nanopores. *J. Phys. Chem. B*, **111**, 2033-2044 (2007)

17. Dong S.-H., Lozada-Cassou M., Yu J., Jiménez-Ángeles F., Rivera A. L.; Hidden Symmetries and Thermodynamic Properties for a Harmonic Oscillator Plus an Inverse Square Potential, *Int. J. of Quant. Chem.*, **107**, 366-371 (2007)
18. Odriozola G., Jiménez-Ángeles F., Lozada-Cassou M.; Effect of Confinement on the Interaction Between Two Like-Charged Rods, *Phys. Rev. Lett.*, **97**, 018102 (2006)
19. Odriozola G., Jiménez-Ángeles F., Lozada-Cassou M.; Two Rods Confined by Positive Plates: Effective Forces and Charge Distribution Profiles, *J. Phys.: Cond. Matt.*, **18**, S2335-S2352 (2006)
20. Jiménez-Ángeles F., Gerardo Odriozola, Lozada-Cassou M.; Electrolyte Distribution Around two Like-Charged Rods and Their Effective Attractive Interaction, *J. Chem. Phys.*, **124**, 134902 (2006)
21. Jiménez-Ángeles F., Lozada-Cassou M.; A Simple model for a Semi-Permeable Membrane: Donnan Equilibrium; *J. Phys. Chem. B*, **108**, 1719-1729 (2004)
22. Jiménez-Ángeles F., Lozada-Cassou M.; A Model Macroions Solution Next to a Charged Wall: Charge Reversal, Charge Inversion and Overcharging by Macroions; *J. Phys. Chem. B*, **108**, 7286-7296, (2004)
23. Gonzalez-Tovar E., Jiménez-Ángeles F., Messina R., Lozada-Cassou M.; A New Correlation Effect in the Helmholtz and Surface Potentials of the Electrical Double Layer; *J. Chem. Phys.* **120**, 9782-9792, (2004)
24. Jiménez-Ángeles F., Lozada-Cassou M.; Overcharging by Macroions: Above All an Entropy Effect; *Coloides e interfaces (Universidad de Vigo, Spain)*; **42**, 159-164 (2003)
25. Jiménez-Ángeles F., Messina R., Lozada-Cassou M. and Holm C.; Ion Pairing in Model Electrolytes: A Study Via Three Particle Correlation Functions; *J. Chem. Phys.*, **119**, 4842-4856 (2003)
26. Deserno M., Jiménez-Ángeles F., Holm C., Lozada-Cassou M., Overcharging of DNA in the Presence of Salt: Theory and Simulation; *J. Phys. Chem. B*, **105**, 10983-10991 (2001)
27. M. Fernández, L. A. Julio Sánchez, S. Camacho López, C. García, E. Haro Poniowski, M. A. Camacho, Jiménez, M. Camacho López, R. Cortez, L. Dagdug, C. Díaz, I. A. Mayen, S. Mera, J. F. Mercado, O. Reséndis, U. Ruiz, C. A. Tapia, S. Trejo, F. Patiño, P. J. Sierra; Los láseres en la UAM, *Revista Contactos* (publicado por Universidad Autónoma Metropolitana, México D.F., México), Vol. 7, Págs. 5-12 (1995).
28. M. Fernández, L. A. Julio Sánchez, S. Camacho López, C. García, E. Haro Poniowski, M. A. Camacho, F. Jiménez, M. Camacho López, R. Cortez, L. Dagdug, C. Díaz, I. A. Mayen, S. Mera, J. F. Mercado, O. Reséndis, U. Ruiz, C. A. Tapia, S. Trejo, F. Patiño, P. J. Sierra; Los láseres en la UAM-II, *Revista Contactos* (publicado por Universidad Autónoma Metropolitana, México D.F., México), Vol. 8, Págs. 7-12 (1995).
29. Felipe Jiménez-Ángeles, Estudio de la interfase de una membrana semipermeable: Donnan Equilibrium (A study of the interface of a semipermeable membrane: Donnan Equilibrium), M. D. Thesis, Universidad Autónoma Metropolitana-Iztapapapa, México D. F., 1998
30. Felipe Jiménez-Ángeles, Efectos entrópicos y de correlaciones de largo alcance en fluidos cargados complejos (Entropy effects and long range correlations in complex charged fluids), Ph.D. Thesis, Universidad Autónoma Metropolitana-Iztapapapa, México D. F., 2002

CONFERENCE PROCEEDINGS

1. Jiménez-Ángeles F., Firoozabadi A. Nucleation Pathways and Interfacial Properties of Methane Hydrates From Molecular Dynamics Simulations; Proceedings of the 8th International Conference on Gas Hydrates (ICGH8-2014), Beijing, China, 28 July - 1 August, 2014
2. Jiménez-Ángeles F., Population inversion as a separation method of two mixed fluids; Memorias del 2do. Congreso Nacional de Membranas: Ciencia, Tecnología y Aplicaciones, June 27 and 28 2011, Facultad de Química UNAM

UNPUBLISHED WORKS

- Jiménez-Ángeles F and Lozada-Cassou M., The Effect of Entropy on Macroions adsorption, unpublished work (2003), see <http://arxiv.org/abs/cond-mat/0303519>
- Jiménez-Ángeles, Messina R., González-Tovar E., Lozada-Cassou M., Ion Distribution, Mean Electrostatic Potential and Differential Capacity for a Highly Concentrated Electrolyte Near a Charged Wall, unpublished
- Odriozola G., Orea P., Jiménez-Ángeles F., Assisted Crystal Growing by Tempering Metastable Vapor-Liquid Fluids; see <http://arxiv.org/pdf/1010.5261.pdf>

TALKS AT CONFERENCES

1. Hydrate Molecular Structures By Molecular Dynamics Simulations and Thermodynamic Stability Analysis, XIV AIChE Annual Meeting, Atlanta, USA, 2014
2. Ionic Adsorption on Charged Surfaces of Different Geometries, Mexicana Meeting On Theoretical Physical Chemistry, Pachuca, Mexico, 2011
3. The ζ -potential for a Concentrated Colloidal Dispersion: The Colloidal Primitive Model vs. the Cell Model, ELKIN, Turku, Finland, 2010
4. The Regimes of Charge Reversal, XVII Meeting on Science and Technology of Complex Fluids, San Luis Potosí, Mexico, 2004
5. On the Regimes of Charge Reversal, Applied Statistical Physics, organized by The Mexican Academy on Molecular Engineering, Puerto Vallarta, Mexico, 2003

POSTERS AT CONFERENCES

1. Jiménez-Ángeles F., Charge Reversal at the Electrical Double Layer Produced by Mixed Discrete Surface Charges, Mexican Meeting on Theoretical Physical Chemistry, Toluca Mexico, 2012
2. Jiménez-Ángeles F., The Electrical Double Layer Produced by Mixed Discrete Surface Charges, 4th Meeting on Molecular Simulations: From Simple Fluids to Chemical Reactions, Mexico City, 2012
3. Jiménez-Ángeles F. and M. Lozada, Electrokinetic Properties of Size-Asymmetric Electrolytes Confined in a Slit Nanopore, ELKIN, Turku, Finland, 2010

4. Jiménez-Ángeles F. and M. Lozada, A Theoretical Study of the Adsorption of Macroions on a Charged Surface, CIASEM, Veracruz, Mexico, 2001
5. Jiménez-Ángeles F. and M. Lozada, Self Assembling of Macroions in a Slit Pore, Applied Statistical Physics, organized by The Mexican Academy on Molecular Engineering, Cancún, Mexico, 2001
6. Jiménez-Ángeles F. and M. Lozada, The Overcharging Effect, XXX Winter Meeting on Statistical Physics, Taxco, Mexico, 2001
7. Gabriel E. Aguilar-Pineda, Felipe Jiménez-Ángeles and M. Lozada, The Semipermeable Cylindrical Pore, XII Meeting on Science and Technology of Complex Fluids, San Luis Potosi, Mexico, 1999
8. F. Jiménez-Ángeles and M. Lozada, The Semipermeable Membrane, XII Meeting on Science and Technology of Complex Fluids, San Luis Potosi, Mexico, 1999
9. F. Jiménez-Ángeles and M. Lozada, The Semipermeable Membrane: Donan Equilibrium, 4th Liquid Matter Conference, Granada Spain, 1999
10. F. Jiménez-Ángeles and M. Lozada, The Semipermeable Membrane, XXV Winter Meeting on Statistical Physics, Cuernavaca, Mexico, 1998

TALKS AND SEMINARS

1. Molecular Dynamics Simulations of Hydrates, XXIV Annual Workshop, Reservoir Engineering Research Institute, May 9-10, 2013.
2. Charge Reversal at the Electrical Double Layer Produced by Mixed Discrete Surface Charges, Séminaire de Physique, Institut de Chimie, de Physique et des Matériaux, Université de Lorraine, Metz France, June 29, 2012
3. Polarity Inversion of ζ -potential in Concentrated Colloidal Dispersion, at Institut für Theoretische Physik II, Heinrich-Heine-Universität, Düsseldorf, Germany, October 2010
4. Resultados de las Teorías de Líquidos en Sistemas Coloidales, Seminar of the Area of Materials and Nanostructures of the graduate program, Mexican Petroleum Institute, Mexico City, March 2004
5. The Overcharging Effect on the Formation of Nanostructures, Seminar of the Molecular Engineering Program, Mexican Petroleum Institute, Mexico City, December 2000
6. Three particle Correlation Function for an Electrolyte, at 2nd Symposium on Chemical Physics of Fluids, Area of Physics of Liquids, Universidad Autónoma Metropolitana, April 2000
7. Structure of a Complex Fluid in Pores and Walls and Its Biophysical Implications; Seminarios of the Biomedical Engineering Area, Universidad Autónoma Metropolitana, July 1999

SUPERVISION OF THESIS

- H. M. Manzanilla, Statistical Mechanics of Concentrated Colloidal Dispersions, Ph. D. Thesis, Instituto Mexicano del Petróleo, 2011

- J. A. González, A Theory of Size Asymmetric Charged Fluids Applied to a Simple Model of the DNA Electrolyte Environment
M. Sc. Thesis, Institute of Physics and Mathematics, Universidad Michoacana de San Nicolás de Hidalgo, 2006

REVISION OF THESIS

- H. M. Manzanilla-Granados, Study of the Electrophoretic Mobility Via the Standard and Primitive Models of Electrophoresis, M. Sc. Thesis, School of Physics and Mathematics, Instituto Politécnico Nacional, 2006
- E. Sánchez Arellano, Electrokinetic and Structural Properties of Electrolytes Confined in Cylindrical and Slit-Like Nanopores, Ph. D. Thesis, Department of Physics, Universidad Autónoma Metropolitana-Iztapalapa, 2010

AWARDS AND FELLOWSHIPS

1. National Researcher Level 2 by National System of Researchers since 2013, CONACYT Mexico.
2. National Researcher Level 1 by National System of Researchers from 2006 to 2012, CONACYT Mexico.
3. Candidate to National Researcher by National System of Researchers from 2003 to 2005, CONACYT Mexico.
4. University Medal for outstanding performance in the Master studies at Universidad Autónoma Metropolitana, 1998
5. University Medal for outstanding performance in Ph. D. studies at Universidad Autónoma Metropolitana, 2002
6. Graduate Fellowship from CONACYT for Master in Science studies, Universidad Autónoma Metropolitana Campus Iztapalapa, Mexico City, 1996-1998
7. Graduate Fellowship from CONACYT for Ph. D. studies, Universidad Autónoma Metropolitana Campus Iztapalapa, Mexico City, 1998-2002
8. Research grant from Instituto Mexicano del Petroleo from 2001-2002, Mexico. from 1996 to 1998
9. Graduate Fellowship from NEGROMEX Industries for Ph. D. studies, Universidad Autónoma Metropolitana Campus Iztapalapa, Mexico City, 1998-2001
10. Research grant from the National Council for Science and Technology (CONACYT) and National System of Researchers (SNI), Mexico. from 1996 to 1998

SCIENTIFIC SOCIETIES AND MEMBERSHIPS

- Member of National System of Researchers, CONACYT Mexico
- Member of the American Institute of Chemical Engineers (AIChE)
- Founder Member of the Mexican Society of Science and Technology of Membranes

- Founder Member of the Mexican Academy of Molecular Engineering

RESEARCH INTERESTS

My research interest is in Statistical Physics, Complex Fluids and Soft Matter. This includes electrolytes, polyelectrolytes, colloidal suspensions, macromolecules, hydrocarbon fluids. I have studied models of complex fluids by means of Integral equations theories and computer simulations. Specifically I am interested in

- Hydrate nucleation and growth
- Interfacial phenomena of hydrates
- Molecular mechanisms of hydrate antiagglomeration and inhibition
- Interaction of liquid hydrocarbons/aqueous solutions/mineral substrates
- Adsorption phenomena
- Molecular recognition and self-assembling
- Statistical mechanics of concentrated colloidal dispersions
- Confinement of complex fluids in nanopores
- Effective interactions between colloidal particles: Effects of confinement, charge, entropy
- Phase transitions of confined complex fluids
- Electrokinetic properties of electrolytes in nanopores

LANGUAGES

ENGLISH: Fluent
SPANISH: Mother tongue
FRENCH: Basic Knowledge

INTERESTS AND ACTIVITIES

Technology, Programming
Photography, Travelling