

FLOR REBECA SIPERSTEIN

Personal information

Nationality: Mexican
Female, date of birth 15/07/1971

Current position

Research Professor
Departament d'Enginyeria Química
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Education

1995-2000	University of Pennsylvania PhD Chemical Engineering Advisors: Prof. Alan L. Myers and Raymond J. Gorte	Philadelphia, PA
1990-1994	Universidad Nacional Autónoma de México BS Chemical Engineering (Mención honorífica) Advisor: Prof. Enrique Bazúa Rueda	México, D.F.

Research Experience

2003-	Universitat Rovira i Virgili Research Professor Complex Systems Group •Surfactant self-assembly and phase behaviour •Formation of porous materials •Behaviour of confined fluids	Tarragona, Spain
2002	Université de Paris Sud XI Laboratoire de Chimie Physique Visiting scientist (3 months) •Freezing of fluids in MCM-41 type materials using molecular simulation	Orsay, France
2000-2002	North Carolina State University Postdoctoral Researcher •Modeling the formation of porous materials using surfactant templating •Modeling adsorption and freezing in MCM-41 type materials	Raleigh, NC
1995-2000	University of Pennsylvania Graduate researcher •Mixture adsorption in zeolites •Molecular modeling of adsorption of gases in zeolites •Volumetric and calorimetric measurements for mixture adsorption	Philadelphia, PA

Teaching Experience

2003-2004	Universitat Rovira i Virgili • Enginyeria Química (Mass and Energy Balances) 60 hours • Termodinámica Técnica I (Thermodynamics) 30 hours • Thesis project 10 hours • Laboratori d'Investigació (undergraduate research project) 5 students	Tarragona, Spain
2000-2002	North Carolina State University Invited lectures •ChE 713 Lecture on Molecular Modeling (Prof. responsible: Orlin Velev, Fall 2001) •ChE 714 Lecture on Modeling of Surfactants (Prof. responsible: Keith Gubbins, Spring 2000) •ChE 713 Lecture on Properties of Solutions (Prof. responsible: Keith Gubbins, Fall 2000)	Raleigh, NC
1995-2000	University of Pennsylvania Teaching assistant •ChE-231 Thermodynamics (30 hours approx) •Chem-101 Freshmen Chemistry (30 hours approx) •Math-130 Freshmen Calculus (90 hours approx)	Philadelphia, PA
1995-2000	Universidad Nacional Autónoma de México Teaching assistant •Thermodynamical properties •Mass and Energy Balances	México, D.F.

Other

- Praxair Award 1999 (AIChE Separations Division Graduate Research Award in Adsorption and Ion Exchange)
- Editor's choice (AIChE J. May 2001). Paper reviewed in 'Understanding adsorption of nonideal mixtures', Chem. Eng. Progress, 22, (May, 2001)
- Reviewer for Fluid Phase Equilibria and Journal of Physical Chemistry B.

Publications

1. S. Savitz, F. Siperstein, R.J. Gorte, A.L. Myers "Calorimetric Study of Adsorption of Alkanes in High-Silica Zeolites" *Journal of Physical Chemistry B* 102, 6865-6872 (1998)
2. S. Savitz, F. Siperstein, R. Huber, S.M. Tieri, R.J. Gorte, A.L. Myers, C.P. Grey, D.R. Corbin "Adsorption of hydrofluorocarbons HFC-134 and HFC-134a on X and Y zeolites: Effect of ion-exchange on selectivity and heat of adsorption" *Journal of Physical Chemistry B* 103, 8283-8289 (1999)
3. F. Siperstein, R.J. Gorte and A.L. Myers "Measurement of Excess Functions of Binary Gas Mixtures Adsorbed in Zeolites by Adsorption Calorimetry" *Adsorption*, 169-176 (1999)
4. F. Siperstein, R.J. Gorte and A.L. Myers "A New Calorimeter for Simultaneous Measurements of Loading and Heats of Adsorption from Gaseous Mixtures" *Langmuir*, 1570-1576 (1999)
5. D.M. Shen, M. Bulow, F. Siperstein, M. Engelhard, A.L. Myers "Comparison of experimental techniques for measuring isosteric heat of adsorption" *Adsorption* 6, 275-286 (2000)
6. F.R. Siperstein, A.L. Myers "Mixed-gas adsorption" *AIChE J.* 47(5), 1141-1159 (2000)
7. A.L. Myers, F.R. Siperstein "Characterization of adsorbents by energy profile of adsorbed molecules" *Colloids and Surfaces A*, 187-188, 73-81 (2001)

8. F.R. Siperstein, K.E. Gubbins "Synthesis and characterization of templated mesoporous materials using molecular simulation" *Molecular Simulation* 27(5-6) 339-352 (2001)
9. F. Siperstein, A.L. Myers, O. Talu "Long range corrections for computer simulations of adsorption" *Molecular Physics*(13), 2025-2030 (2002)
- 10.C.M. Colina, M. Lisal, F.R. Siperstein, K.E. Gubbins "Accurate CO₂ Joule-Thomson inversion curve by molecular simulations" *Fluid Phase Equilibria*202(2), 253-262 (2002)
- 11.F.R. Siperstein, K.E. Gubbins "Influence of synthesis conditions on surface heterogeneity of M41 type materials studied with lattice Monte Carlo" *Studies in Surface Science and Catalysis* 144, 647-654 (2002)
- 12.F.R. Siperstein, K.E. Gubbins "Phase separation and liquid crystal self-assembly in surfactant-inorganic-solvent systems" *Langmuir*19(6) 2049-2057 (2003)
- 13.C.M. Colina, C.G. Olivera-Fuentes, F.R. Siperstein, M. Lisal, K.E. Gubbins "Thermal properties of supercritical carbon dioxide by Monte Carlo simulations" *Molecular Simulation*29(6-7) 405-412 (2003)
- 14.M. Lisal, J.K. Brennan, W.R. Smith, F.R. Siperstein "Molecular simulation of reaction and adsorption in nanochemical devices. Increase of reaction conversion by separation of a product from the reaction mixture" *Journal of Chemical Physics* 121(10), 4901-4912 (2004)
- 15.F.R. Siperstein "Determination of Azeotropic behavior in Adsorbed Mixtures" *Adsorption* 11, 55-59 (2005)
- 16.F.R. Hung, E.E. Santiso, B. Coasne, K.E. Gubbins, F.R. Siperstein, M. Sliwinska-Bartkowiak "Effect of confinement on freezing of CCl₄ in cylindrical pores" *Adsorption* 11, 391-396 (2005)
- 17.N. Chennamsetty, H. Bock, L.F. Scanu, F.R. Siperstein, and K.E. Gubbins "Cosurfactant and cosolvent effects on surfactant self-assembly in supercritical carbon dioxide" *Journal of Chemical Physics* 122, 094710 (2005)
- 18.F.R. Hung, B. Coasne, E.E. Santiso, K.E. Gubbins, F.R. Siperstein, M. Sliwinska-Bartkowiak "Molecular modelling of freezing of simple fluids confined within carbon nanotubes" *Journal of Chemical Physics* 122, 144706 (2005)
- 19.B. Coasne, F.R. Hung, F.R. Siperstein, K.E. Gubbins, "Molecular simulation of gas adsorption in realistic models of silica nanopores" *Annales de Chimie-Science des Matériaux*, 30(4) 375-383 (2005)
- 20.B. Coasne, F.R. Hung, R.J.-M. Pellenq, F.R. Siperstein, K.E. Gubbins, "Adsorption of Simple Gases in MCM-41 Materials: The Role of Surface Roughness" *Langmuir*, in press
- 21.F.R. Siperstein and A.D. Macke "Phase behaviour of a model surfactant/solvent system at intermediate and high density" *Colloids and Surfaces A, Physicochemical and Engineering Aspects*, in press.
- 22.A. Patti, A.D. Mackie and F.R. Siperstein "Molecular simulation study on the structure of templated porous materials obtained from different inorganic precursors" *Studies in Surface Science and Catalysis* in press.
- 23.V. Fierro, G. Bosch and F.R. Siperstein "PSD obtained from molecular modelling and DFT in microporous carbons" *Studies in Surface Science and Catalysis* in press.
- 24.F.R. Hung, B. Coasne, K.E. Gubbins, F.R. Siperstein and M. Sliwinska-Bartkowiak "A Monte Carlo study of capillary condensation of krypton within realistic models of templated mesoporous silica materials" *Studies in Surface Science and Catalysis* in press.
- 25.A. Patti, A.D. Mackie and F.R. Siperstein "Monte Carlo simulation of self-assembled ordered hybrid materials" *Langmuir* submitted 2005.

Refereed conference proceedings

1. F. Siperstein, R.J. Gorte, A.L. Myers "Experimental studies of adsorption of mixtures in zeolites using microcalorimetry" *Proceedings of the Twelfth International Zeolite Conference* 102-109 (1998)
2. F. Siperstein, S. Savitz, R.J. Gorte, A.L. Myers "Microcalorimetric Characterization of Zeolites Using Polar and Nonpolar Probe Molecules" *Fundamentals of Adsorption - FOA6* 111-116 (1998)
3. F. Siperstein, A.L. Myers "Effect of Temperature on Adsorption Equilibria of Gas Mixtures" *Fundamentals of Adsorption - FOA6* 57-62 (1998)
4. D.M. Shen, M. Engelhard, F. Siperstein, A.L. Myers, M. Bulow "Comparison of sorption heats from isosteric and calorimetric experiments for nitrogen, oxygen and carbon dioxide on zeolites of types LTA and FAU" *Adsorption Science and Technology* 106-110 (2000)
5. F. Siperstein, A.L. Myers, O. Talu "Gas storage: Absolute adsorption versus excess adsorption" *Fundamentals of Adsorption* 7, 311-318 (2001)
6. F. Siperstein, K.E. Gubbins "Mimetic Synthesis of Templated Mesoporous Materials using Molecular Simulation" *Fundamentals of Adsorption* 7, 434-440 (2001)

Presentations and Posters

1. Siperstein, F.; Savitz, S.; Gorte, R.J.; Myers A.L. "Experimental Measurements of Mixture Equilibria and Heats of Adsorption on Zeolites" NECZA Meeting (Poster) Philadelphia, PA 1997.
2. Myers, A.L.; Gorte, R.J.; Dunne, J.A.; Savitz, S.; Siperstein, F. "Experimental Data on Excess Free Energy and Excess Enthalpy of Binary Gas Mixtures Adsorbed in Zeolites" AIChE Annual Meeting (Oral) Los Angeles, CA 1997
3. Siperstein, F.; Gorte, R.J.; Myers A.L. "Experimental Studies of Adsorption of Mixtures in Zeolites using Microcalorimetry" 12th International Zeolite Conference (Oral) Baltimore, MD 1998
4. Siperstein, F.; Savitz, S.; Gorte, R.J.; Myers A.L. "Microcalorimetric Characterization of Zeolites Using Polar and Nonpolar Probe Molecules" Fundamentals of Adsorption 6 (Oral) France 1998
5. Siperstein, F.; Myers A.L. "Effect of Temperature on Adsorption Equilibria of Gas Mixtures" Fundamentals of Adsorption 6 (Oral) France 1998
6. Siperstein, F.; Myers A.L.; Talu, O. "Binary Mixture Adsorption in Zeolites: A comparison between experiment and molecular simulation" NECZA Meeting (Poster) Philadelphia, PA 1999
7. Myers, A.L.; Siperstein, F. "Adsorption in Zeolites: Loading, Heats, and Entropies of Pure and Mixed Gases" AIChE Annual Meeting, Dallas, TX (Oral) 1999
8. Siperstein, F.; Myers, A.L. "Adsorption of Gas Mixtures on Zeolites" AIChE Annual Meeting, Dallas, TX (Oral, Plenary) 1999
9. Siperstein, F.; Myers, A.L., Talu, O. "Understanding non-ideal Mixture Adsorption using Molecular Simulation" Gordon Research Conference on Separations and Purification, New London, NH (Poster) 2000
10. Siperstein, F.; Myers, A.L., Talu, O. "Long-Range Corrections for Energy and Amount Adsorbed in Zeolites" AIChE Annual Meeting, Los Angeles, CA (Oral) 2000
11. Siperstein, F.; Myers, A.L., Talu, O. "Gas storage: Absolute Adsorption versus Excess Adsorption" Fundamentals of Adsorption 7, Nagasaki, Japan (Oral) 2001
12. Siperstein, F.; Gubbins, K.E. "Mimetic Synthesis of Templated Mesoporous Materials using Molecular Simulation" Fundamentals of Adsorption 7, Nagasaki, Japan (Poster) 2001
13. Fillous, L.H.; Siperstein, F.; Lisal, M.; Gubbins, K.E. "Phase Behavior of Water/Oil/Surfactant Systems (WOS) using lattice Monte Carlo. Determination of Optimum Formulation" AIChE Annual Meeting, Reno, NV (Oral) 2001
14. Siperstein, F.; Gubbins, K.E. "Mimetic Synthesis and Characterization of Templated Mesoporous Materials Using Molecular Simulation" AIChE Annual Meeting, Reno, NV (Oral) 2001
15. Siperstein, F.; Gubbins, K.E. "Influence of the synthesis conditions on surface heterogeneity of M41 type materials studied with lattice Monte Carlo" COPS VI - Characterization of Porous Solids (Poster) Alicante (ESPAÑA) 2002
16. Siperstein, F.; Gubbins, K.E. "Liquid Crystal Self-assembly of Surfactant-inorganic Oxide Systems using Monte Carlo Simulations" AIChE Annual Meeting, Indianapolis, IN (Oral) 2002
17. Hung, F. R.; Siperstein, F. R.; Sliwiska-Bartkowiak, M.; Alba-Simionesco C.; Gubbins, K.E. "Freezing/melting behavior of fluids confined in carbon nanotubes and MCM-41: simulations and experiments" AIChE Annual Meeting, Indianapolis, IN (Oral) 2002
18. Colina, C.M.; Olivera-Fuentes, C. G.; Lisal, M.; Siperstein, F.R.; Gubbins, K.E. "Thermal Properties of Carbon Dioxide in the Single Phase Region by Monte Carlo Simulations" AIChE Annual Meeting, Indianapolis, IN (Poster) 2002
19. Colina, C.M.; Lisal, M.; Siperstein, F.R.; Gubbins, K.E. "Accuracy of Joule-Thomson Inversion Curves by Molecular Simulation" Sixth Liblice Conference on the Statistical Mechanics of Liquids, Spindleruv Mlyn, Czech Republic (Poster) 2002
20. Bock, H.; Siperstein, F.R.; Gubbins, K.E. "Hydrogen-Bonds in Lattice Monte Carlo Simulations of Surfactants" FOMMS 2003, Keystone Resort, CO (Poster) 2003
21. Siperstein, F.R.; Gubbins, K.E. "Phase behavior of surfactant-inorganic oxides liquid crystals" FISES 2003, Pamplona, Spain (Oral) 2003
22. Siperstein, F.R. "Simulation of argon, krypton and nitrogen adsorption in silicalite" FISES 2003. Pamplona, Spain (Poster) 2003
23. Siperstein, F.R. "Determination of Azeotropic Behaviour in Adsorbed Mixtures" Fundamentals of Adsorption 8, Sedona, AZ (Oral, Plenary) 2004

- 24.F.R. Hung, E.E. Santiso, B. Coasne, K.E. Gubbins, F.R. Siperstein, M. Sliwinska-Bartkowiak "Effect of confinement on freezing in cylindrical pores" Fundamentals of Adsorption 8, Sedona, AZ (Poster) 2004
- 25.Siperstein, F.R.; Mackie, A.D. "Simulation of Surfactants at Intermediate and High Densities" 18th Conference of the European Colloid and Interface Society, Almería, Spain (Poster) 2004
- 26.Siperstein F.R., Bladé M. "GCMC simulation of nitrogen in porous carbons" XXIX Reunión Ibérica de Adsorción, Oporto, Portugal (Poster) 2004
- 27.Patti, A. Mackie A.D. and F.R. Siperstein "Molecular simulation study on the structure of templated porous materials obtained from different inorganic precursors" Characterization of Porous Solids VII, Aix en Provence (Poster) 2005.
- 28.Fierro, V. Bosch G. and F.R. Siperstein "PSD obtained from molecular modelling and DFT in microporous carbons" Characterization of Porous Solids VII, Aix en Provence (Poster) 2005.
- 29.Hung, F.R. Coasne, B. Gubbins, K.E. Siperstein F.R. and M. Sliwinska-Bartkowiak "A Monte Carlo study of capillary condensation of krypton within realistic models of templated mesoporous silica materials" Characterization of Porous Solids VII, Aix en Provence (Poster) 2005
- 30.Gomez Mendez, G. Pérez-Pellitero, J. Siperstein, F.R. and A.D. Mackie "Determinación de propiedades de equilibrio para tiofenos mediante simulación molecular" XIII Congreso de Física Estadística FISES 05, Madrid (Poster) 2005
- 31.Patti, A. Mackie, A.D. and F.R. Siperstein "Molecular Modelling of Hybrid Materials" XIII Congreso de Física Estadística FISES 05, Madrid (Poster) 2005
- 32.Patti, A. Mackie A.D. and F.R. Siperstein "Self assembly of ordered organic-inorganic materials" AIChE Annual Meeting, Cincinnati, OH (Oral) 2005.
- 33.Bosch G. Lisal, M. and F.R. Siperstein "Adsorption of nitrogen and methane in ETS-4" AIChE Annual Meeting, Cincinnati, OH (Oral) 2005.

Invited presentations

- "Prediction of Nonideal Gas Mixture Adsorption" Department of Chemical Engineering, University of Virginia, Charlottesville, VA (USA) 30/03/2000
- "Simulation of Surfactant Templated Nanoporous Materials" Department of Chemical Engineering, Yale University, New Haven, CT (USA) 27/02/2002
- "Surfactant templated nanoporous materials", Chimie de la Matière Condensée, Université Pierre et Marie Curie, Paris, (France) 27/03/2002
- "Adsorption of Gas Mixtures on Zeolites" Molecular Modelling group (Professors B. Smit y R. Krishna), Chemical Engineering Department, University of Amsterdam 19/04/2002
- "Adsorption of nitrogen and methane in titanosilicates" CECAM workshop "Towards new methods to design catalytic and separation processes in nanoporous materials" Lyon, 2005
- "Aplicaciones de modelado molecular en el estudio de adsorción en materiales porosos" Laboratorio de Materiales Avanzados (Prof. Francisco Rodríguez Reinoso), Departamento de Química Inorgánica, Universidad de Alicante, Alicante 25/11/2005.

Funding and Research Projects

Title: Nanoreactors Modelling and Simulation: Ajut per a l'elaboració d'un projecte europeu (STREP) de l'àrea del 6è. Programa Marc

Program: Accions especials de recerca (ACES) Direcció General de Recerca, Generalitat de Catalunya

PI F.R. Siperstein. Duration 2004

Amount: 1000.00 €

Title: Materiales híbridos orgánico-inorgánicos

Program: Accions integrades (ACI), Direcció General de Recerca, Generalitat de Catalunya

PI F.R. Siperstein. Duration 2004-2006

Amount: 4850.00 €

Title: Predicción de propiedades termofísicas de mezclas de fluidos complejos.

Proyecto de I+D+I, Ministerio de Ciencia y Tecnología

PI J. Bonet Avalos. Duration 2004-2007

Amount: 65,000.00 €

Title: ALFA II 0412FAFI LIGNOCARB Lignin and derived carbonaceous materials for gas storage and environmental applications

Europa Aid Cooperation Office

PI V. Fierro. Duration 2005-2008

Amount: 687,999.20 € (EU contribution 515,999.40 €)

Title: BE 00334 Separación de nitrógeno y metano mediante adsorción en titanosilicatos

Direcció General de Recerca, Generalitat de Catalunya

PI F.R. Siperstein. Duration 2005-2006

Amount: 1,930 €

Title: DESANNS: Advanced separation and storage of carbon dioxide: Design, Synthesis, and Applications of Novel Nanoporous Sorbents

FP6-2004-Energy-3 SUSDEV-1.2.7

Project Coordinator P. Llewellyn (CNRS), URV Coordinator F.R. Siperstein. Duration 2006-2009

Amount: 2.5M € (URV budget 260,004 €)

Title: OPEN ToK: On Process and Engineering of Nanoporous materials Transfer of Knowledge

FP6-2004 -Mobility-3

PI F.R. Siperstein. Duration 2006-2010

Amount: in negotiation (Requested 700,000 €)
