

## Publications

S. Figueroa-Gerstenmaier, J. Bonet Avalos, L. D. Gelb, K. E. Gubbins, L. F. Vega.  
“Pore Size Distribution of Porous Glasses: A Test of the Independent Pore Model.”  
*Langmuir*, **19**, 8592-8604 (2003).

S. Figueroa-Gerstenmaier, V. Fierro.  
“Use of density functional theory in determining pore size distributions of activated carbons prepared from Kraft lignin.”  
*Proceedings of “Carbon 2003”* Oviedo, Spain, 2003.

S. Figueroa-Gerstenmaier, F. J. Blas, J. Bonet Avalos, L. F. Vega.  
“Application of the fundamental measure density functional theory to the adsorption in cylindrical pores.”  
*J. Chem. Phys.*, **118**, 830-842 (2003).

S. Figueroa-Gerstenmaier, L. F. Vega, F. J. Blas, K. E. Gubbins.  
“Molecular model of  $\gamma$ -alumina: nitrogen adsorption and pore size distribution.”  
*AIChE Symposium Series No. 325*, **97**, 317-320 (2001).

S. Figueroa-Gerstenmaier, F. J. Blas, L. F. Vega.  
“Isotermas de adsorción en  $\gamma$ -alúmina mediante simulación molecular.”  
*Proceedings of “II Jornadas Nacionales de Ingeniería Termodinámica”*, p. 266-273. Tarragona, Spain, 2001.

S. F. Gerstenmaier, F. J. Blas, K. E. Gubbins, L. F. Vega.  
“Modelado molecular de alúmina para procesos de separación. Comparación entre teoría, simulación, y datos experimentales”.  
*Proceedings of “I Jornadas Nacionales de Ingeniería Termodinámica”*, p. 344. Badajoz, Spain, 1999.

S. Figueroa-Gerstenmaier, A. Cabañas, M. Costas.  
“Self-association and complex formation in alcohol-unsaturated hydrocarbons systems. Heat capacities of linear alcohols mixed with alkenes and alkynes”. *PCCP* **1**, 665-674 (1999).

E. Barberà, M. B. Molins, M. J. Moya, R. Grau, A. Porta, S. Figueroa.  
“Seguimiento de procesos fermentativos: medida de la concentración de glucosa mediante un sistema FIA no enzimático”.  
*Afinidad*, **50** (448), 378-382 (1993).

S. Figueroa-Gerstenmaier, F. Medina, F. J. Blas, L. F. Vega.  
“Pore size distribution of  $\gamma$ -alumina by adsorption of nitrogen and density functional theory.” In preparation.

S. Figueroa-Gerstenmaier, J. Bonet Avalos.  
“Pore-size distributions of materials from Density Functional Theory. Modelling of porous glasses as a combination of independent slit-like and cylindrical pores.” In preparation.

S. Figueroa-Gerstenmaier, M. Lisal.  
“Reaction and Osmotic Equilibria: Molecular Simulation of Methanol Reforming in Supercritical Water”. In preparation.

## Contributions to conferences

S. Figueroa-Gerstenmaier, V. Fierro.  
“Use of density functional theory in determining pore size distributions of activated carbons prepared from Kraft lignin”.  
Poster in Carbon 2003. Oviedo, Spain, 2003.

C. Herdes, S. Figueroa-Gerstenmaier, F. Medina, L. F. Vega.  
“Modeling and characterization of adsorbent materials by GCMC simulations and experiments”.  
Oral presentation in the conference Thermodynamics 2003. Cambridge, UK, 2003.

- S. Figueroa-Gerstenmaier, F. J. Blas, J. Bonet Avalos, L. F. Vega.  
“Adsorption behavior of nitrogen in cylindrical and slit-like pores by density functional theory and Monte Carlo simulations”.  
Poster in 9<sup>o</sup> Mediterranean Congress of Chemical Engineering. Barcelona, Spain, 2002.
- S. Figueroa-Gerstenmaier, J. Bonet Avalos, L. D. Gelb, K. E. Gubbins, L. F. Vega.  
“Pore size distribution of model porous glasses by adsorption of nitrogen using density functional theory.”  
Poster in 9<sup>o</sup> Mediterranean Congress of Chemical Engineering. Barcelona, Spain, 2002.
- S. Figueroa-Gerstenmaier, J. Bonet Avalos, F. J. Blas, L. F. Vega.  
“Application of the fundamental measure density functional theory to the adsorption in cylindrical pores. Comparison with molecular simulation”.  
Poster in XI Statistical Physics Meeting (FISES 2002). Tarragona, Spain, 2002.
- S. Figueroa-Gerstenmaier, F. J. Blas, L. F. Vega.  
“Isotermas de adsorción de nitrógeno en  $\gamma$ -alúmina mediante simulación molecular”.  
Poster in II Jornadas de Ingeniería Termodinámica. Tarragona, Spain, 2001.
- S. Figueroa-Gerstenmaier, L. F. Vega, F. J. Blas, L. D. Gelb, K. E. Gubbins.  
“Pore size distribution analysis of model porous glasses by molecular simulation and density functional theory”.  
Oral presentation in American Institute of Chemical Engineers (AIChE) 2000 Annual Meeting. Los Angeles, U.S.A., 2000.
- S. Figueroa-Gerstenmaier, F. J. Blas, K. E. Gubbins, L. F. Vega.  
“Adsorption behaviour and pore size distribution of amorphous materials by density functional theory and Monte Carlo simulation”.  
Poster in X Statistical Physics Meeting (FISES 2000). Santiago de Compostela, Spain, 2000.
- S. Figueroa-Gerstenmaier, L. F. Vega, F. J. Blas, K. E. Gubbins.  
“Molecular model of  $\gamma$ -alumina: nitrogen adsorption and pore size distribution.”  
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- S. Figueroa-Gerstenmaier, F. J. Blas, K. E. Gubbins, L. F. Vega.  
“Grand Canonical Monte Carlo simulations and density functional theory of adsorbent materials.”  
Poster in IX Statistical Physics Meeting (FISES 99). Santander, Spain, 1999.
- S. Figueroa-Gerstenmaier, F. J. Blas, K. E. Gubbins, L. F. Vega.  
“Molecular modeling of alumina for separation purposes. Theory, simulation, and experimental results.”  
Poster in I Jornadas Nacionales de Ingeniería Termodinámica. Badajoz, Spain, 1999.
- S. Figueroa-Gerstenmaier, F. J. Blas, K. E. Gubbins, L. F. Vega.  
“Monte Carlo simulations of adsorption applied to process separation: a comparison with experimental results.”  
Poster in 1998 Conference on Computational Physics. Granada, Spain, 1998.
- Susana Figueroa Gerstenmaier, Miguel Costas  
“Auto asociación de 1-alcoholes en hidrocarburos insaturados.”  
Oral presentation in XII Coloquio Anual de Termodinámica. Mexico, D. F., Mexico, 1997.
- Susana Figueroa Gerstenmaier, Miguel Costas.  
“Self-association of 1-alcohols in unsaturated hydrocarbons.”  
Oral presentation in 2nd International Workshop on VLE and Related Properties in Binary and Ternary Mixtures of Ethers, Alkanes and Alkanols. Valladolid, Spain, 1996.
- Susana Figueroa Gerstenmaier, Vicente Talanquer.  
“Lattice models for micellar solutions with the chemical equilibrium restriction.”  
Poster in XXXV National Congress of Physics. Ensenada, Mexico, 1990.
- Susana Figueroa Gerstenmaier, A. Guzmán-Pérez.  
“An alternative method for the calculation of tetrahedral bond.”  
Oral presentation in IX Congress of Chemical Education. Aguascalientes, Mexico, 1989.

## **Participation in financed projects**

“Development and application of molecular-modelling techniques for the prediction of thermodynamical and transport properties of fluids with industrial importance”.  
(PPQ2001-0671), Minister of Science and Technology, 2001-2004.

“Development and application of molecular-modelling techniques for the prediction of thermodynamical and transport properties of fluids with industrial importance”.  
(PPQ2000-2888-E), Minister of Science and Technology, 2001-2002.

“Molecular modelling of some systems of interest in chemical engineering: adsorption and phase equilibrium”.  
(PB96-1025), DGICYT (Spanish Government), 1997-2000.

“Financial support to the infrastructure for research groups.”  
(2000PIR-21), Universitat Rovira i Virgili, 2000-2001.

“Financial support for research groups to incorporate technical staff.”  
(2000PSR-86), Universitat Rovira i Virgili, 2000-2001.

“Financial support for research groups to incorporate technical staff.”  
(1999PSR-26), Universitat Rovira i Virgili, 1999-2000.

“Molecular modelling of the self-assembly of micelles: Transition between spheres and cylinders”.  
(HI1998-0193), Minister of Education and Culture (Spanish Government), 1999-2000