

## Keith Gubbins

Alba-Simionescu, B. Coasne, G. Dosseh, G. Dudziak, K.E. Gubbins, R. Radhakrishnan and M. Śliwinska-Bartkowiak, "Effects of Confinement on Freezing and Melting", *Journal of Physics: Condensed Matter*, **18**, R15-R68 (2006). [invited review paper]

Benoit Coasne, Francisco R. Hung, Roland J. –M. Pellenq, Flor R. Siperstein and Keith E. Gubbins, "Adsorption of Simple Gases in MCM-41: The Role of Surface Roughness", *Langmuir*, **22**, 194-202 (2006).

C.M. Colina and K.E. Gubbins, "Vapor-Liquid and Vapor-Liquid-Liquid Equilibria of Carbon Dioxide/n-Perfluoroalkane/n-Alkane Ternary Mixtures", *Journal of Physical Chemistry B*, **109**, 2899-2910 (2005).

J. Pikunic, P. Llewellyn, R. Pellenq and K.E. Gubbins, "Argon and Nitrogen Adsorption in Disordered Nanoporous Carbons: Simulation and Experiment", *Langmuir*, **21**, 4431-4440 (2005).

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).

H. Bock, K.E. Gubbins and K.G. Ayappa, "Solid/Solid Phase Transitions in Confined Thin Films: A Zero Temperature Approach", *Journal of Chemical Physics*, **122**, 094709 (2005).

F.R. Hung, K.E. Gubbins, R. Radhakrishnan, K. Szostak, F. Beguin, G. Dudziak and M. Śliwinska-Bartkowiak, "Freezing/Melting of Lennard-Jones Fluids in Carbon Nanotubes", *Applied Physics Letters*, **86**, 103110 (2005).

H. Bock, J. Pikunic and K.E. Gubbins, "Models of Porous Carbons", to appear in *Adsorption by Carbons*, ed. J.M.D. Tascon, Elsevier Pub. Co., Amsterdam (2005).

B. Coasne and K.E. Gubbins and R.J-M. Pellenq, "Temperature Effect on Adsorption/Desorption Isotherms for a Simple Fluid Confined within Various Nanopores", *Adsorption*, **11**, 289-294 (2005).

B. Coasne, J. Czwartos, F.R., K.E. Gubbins, F.R. Hung and M. Śliwinska-Bartkowiak, "Freezing of Mixtures Confined in a Slit Nanopore", *Adsorption*, **11**, 301-306 (2005).

Striolo, K.E. Gubbins, A.A. Chialvo and P.T. Cummings, "The Effect of Pore Connectivity on Water Adsorption Isotherms in Non-Activated Graphitic Nanopores", *Adsorption*, **11**, 337-341 (2005).

Striolo, P.K. Naicker, A.A. Chialvo, P.T. Cummings and K.E. Gubbins, "Simulated Water Adsorption Isotherms in Hydrophilic and Hydrophobic Cylindrical Nanopores", *Adsorption*, **11**, 397-401 (2005).

E.E. Santiso, A.M. George, M. Sliwinska-Bartkowiak, M. Buongiorno Nardelli and K.E. Gubbins, "Effect of Confinement on Chemical Reactions", *Adsorption*, **11**, 349-354 (2005).

S.K. Jain, J.P. Pikunic, R.J-M. Pellenq and K.E. Gubbins, "Effects of Activation on the Structure and Adsorption Properties of a Nanoporous Carbon using Molecular Simulation", *Adsorption*, **11**, 355-360 (2005).

M. Sliwinska-Bartkowiak, F. R. Hung, E.E. Santiso, B. Coasne, G. Dudziak, F.R. Siperstein and K.E. Gubbins, "Effect of Confinement on Freezing of CCl<sub>4</sub> in Cylindrical Pores", *Adsorption*, **11**, 391-396 (2005).

C.M. Colina, C. Olivera-Fuentes and K.E. Gubbins, "Molecular-Based Equations of State at the Graduate Level", *Chemical Engineering Education*, **39**, 250-257 (2005).

Striolo, A.A. Chialvo, K.E. Gubbins and P.T. Cummings, "Water in Carbon Nanotubes: Adsorption Isotherms and Thermodynamic Properties from Molecular Simulation", *J. Chem. Phys.*, in press (2005).

E.E. Santiso, A.M. George, C.H. Turner, M.K. Kostov, K.E. Gubbins, M. Buongiorno-Nardelli and M. Sliwinska-Bartkowiak, "Adsorption and Catalysis: The Effect of Confinement on Chemical Reactions", *Applied Surface Science*, **252**, 766 (2005).

M. Sliwinska-Bartkowiak, R. Radhakrishnan and K.E. Gubbins, "Quasi-Two-Dimensional Melting in Porous Media: Effect of Multi-layers and Cross-Over in Scaling Behavior", *Physical Review B*, submitted (2005).

F.R. Hung, B. Coasne, E.E. Santiso, K.E. Gubbins, F.R. Siperstein and M. Sliwinska-Bartkowiak, "Molecular Modeling of Freezing of Simple Fluids Confined within Carbon Nanotubes", *Journal of Chemical Physics*, **122**, 144706 (2005).

Coasne, F.R. Hung, F.R. Siperstein and K.E. Gubbins, "Molecular Simulation of Gas Adsorption in Realistic Models of Silica Nanopores", *Annales de Chimie – Science des Materieux*, **30**, 375-383 (2005).

M. Kostov, E.E. Santiso, A.M. George, K.E. Gubbins and M. Buongiorno Nardelli, "Catalytic role of defective carbon substrates in the dissociation of water", *Physical Review Letters*, **95**, 136105 (2005).

J. Czwartos, B. Coasne, K.E. Gubbins, F.R. Hung and M. Sliwinska-Bartkowiak, "Freezing and Melting of Azeotropic Mixtures Confined in Nanopores: Experiment and Molecular Simulation", *Molecular Physics*, **103**, 3103-3113 (2005). [B. Widom Special Issue]

N. Chennamsetty, H. Bock and K.E. Gubbins, "Coarse-Grained Potentials from Widom's Particle Insertion Method", *Molecular Physics*, **103**, 3185-3193 (2005). [B. Widom Special Issue]

Benoit Coasne, Keith E. Gubbins, and Roland J.-M. Pellenq, "Domain theory for capillary condensation hysteresis", *Physical Review B*, **72**, 024304 (2005).

Striolo, K.E. Gubbins, M.S. Gruszkiewicz, D.R. Cole, J.M. Simonson, A.A. Chialvo, P.T. Cummings, T.D. Burchell and K.L. More, "Effect of Temperature on the Adsorption of Water in Porous Carbons", *Langmuir*, in press (2005).

T. Ohba, A. Kondo, H. Noguchi, H. Kajiro, K.E. Gubbins and K. Kaneko, "GCMC Simulation of Dynamic Structural Change of Cu-Organic Crystals with N<sub>2</sub> Adsorption", *J. Experimental Nanoscience*, in press (2005).

L.F. Scanu, K.E. Gubbins and C.K. Hall, "Micellization in Supercritical CO<sub>2</sub>/Surfactant Systems: Effect of Surfactant Head Length and CO<sub>2</sub>-Phobicity", *Journal of Chemical Physics*, submitted (2005).

F.R. Hung, B. Coasne, K.E. Gubbins, F.R. Siperstein, M. Thommes and M. Sliwinska-Bartkowiak, "A Monte Carlo Study of Capillary Condensation of Krypton Within Realistic Models of Templated Mesoporous Silica Materials", *Surface Science & Catalysis*, in press (2005). [Proceedings of COPS VII].

Coasne, J. Czwartos, K.E. Gubbins, F.R. Hung and M. Sliwinska-Bartkowiak, "Confinement Effects on Freezing of Binary Mixtures", *Surface Science & Catalysis*, in press (2005). [Proceedings of COPS VII].

S. Bhattacharya, B. Coasne, F.R. Hung and K.E. Gubbins, "Modeling Triblock Surfactant Templated Mesoporous Silicas (MCF and SBA-15): A Mimetic Simulation Study", *Surface Science & Catalysis*, in press (2005). [Proceedings of COPS VII].

S.K. Jain, J. Fuhr, R.J.-M. Pellenq, C. Bichara and K.E. Gubbins, "Stability of Porous Carbon Structures Obtained from Reverse Monte Carlo using Tight Binding and Bond Order Hamiltonians", *Surface Science & Catalysis*, in press (2005). [Proceedings of COPS VII].

S. Bhattacharya and K.E. Gubbins, "Ultra-Large Mesopores in the Triblock Surfactant-Oil-Water-Inorganic Oxide System: Lattice Monte Carlo Simulations", *J. Chem. Phys.*, in press (2005).

M. Jazdzewska, F.R. Hung, K.E. Gubbins and M. Sliwinska-Bartkowiak, "An Experimental Study of Melting of CCl<sub>4</sub> in Carbon Nanotubes", *Phys. Chem. Chem. Phys.*, in press (2005).

F. Hung, S. Franzen and K.E. Gubbins, "A Graduate Course on Multi-Scale Modeling of Soft Matter", *Chemical Engineering Education*, **38**, Fall Issue, 242-249 (2004).

J.K. Brennan, M. Lisal, K.E. Gubbins and B.M. Rice, "Reaction Ensemble Molecular Dynamics: Direct Simulation of the Dynamic Equilibrium Properties of Chemically Reacting Mixtures", *Physical Review E*, **70**, 061103 (2004).

H. Bock and K.E. Gubbins, "The Impact of Hydrogen Bonding on the Temperature Dependence of Surfactant Self-Assembly and Solubility in Aqueous Solution", *Advances in Science & Technology*, **42**, 573-580 (2004).

Striolo, C.C. Colina, K.E. Gubbins, N. Elvassore and L. Lue, "The Depletion Attraction between Pairs of Colloids in Polymer Solution", *Molecular Simulation*, **30**, 437 (2004).

B. Coasne, K.E. Gubbins, F.R. Hung and M. Sliwinska-Bartkowiak, "Freezing and Melting of Binary Mixtures Confined in a Nanopore", *Molecular Physics*, **102**, 2149-2163 (2004).

Striolo, K.E. Gubbins, A.A. Chialvo and P.T. Cummings, "Simulated Water Adsorption Isotherms in Carbon Nanopores", *Mol. Phys.*, **102**, 243-251 (2004).

F.R. Hung, G. Dudziak, M. Sliwinska-Bartkowiak and K.E. Gubbins, "Freezing/Melting Behavior within Carbon Nanotubes", *Mol. Phys.*, **102**, 223-234 (2004).

L.F. Scanu, C.K. Hall and K.E. Gubbins, "Lattice Monte Carlo Simulations of Phase Separation and Micellization in Supercritical CO<sub>2</sub>/Surfactant System. 1. Effect of CO<sub>2</sub> Density", *Langmuir*, **20**, 514-523 (2004).

H. Bock and K.E. Gubbins, "Inverse Temperature Dependence of Surfactant Adsorption from Aqueous Solutions", *Physical Review Letters*, **92**, issue 13, 135701 (2004).

C.M. Colina, A. Galindo, F.J. Blas and K.E. Gubbins, "Phase Behavior of Carbon Dioxide Mixtures with n-Alkanes and n-Perfluoroalkanes", *Fluid Phase Eqba.*, **222-223**, 77-85 (2004).

T.A. Walker, C.M. Colina, K.E. Gubbins and R.J. Spontak, "Thermodynamics of Poly(dimethylsiloxane)/Poly(ethylmethylsiloxane) (PDMS/PEMS) Blends in the Presence of High-Pressure CO<sub>2</sub>", *Macromolecules*, **37**, 2588-2595 (2004).

M. Śliwinska-Bartkowiak, G. Dudziak, M. Kempniński, W. Kempniński, R. Radhakrishnan, F. Hung and K.E. Gubbins, "Melting/Freezing in Narrow Pores: Dielectric and EPR Studies", in "Nonlinear Dielectric Phenomena in Complex Liquids", eds. S.J. Rzoska and V.P. Zhelezny, Kluwer Academic, pp. 357-366 (2004).

B. Coasne, K. E. Gubbins and R. J. -M. Pellenq, "A Grand Canonical Monte Carlo Study of Adsorption and Capillary Phenomena in Nanopores of Various Morphologies and

Topologies: Testing the BET and BJH Characterization methods", *Particle and Particle Systems Characterization*, **21**, 149-160 (2004).

B. Coasne, J.P. Pikunic, R.J.-M. Pellenq and K.E. Gubbins, "Comparison between Adsorption in Pores of a Simple Geometry and Realistic Models of Porous Materials", *Proceedings of the Materials Research Society*, **790**, P8.5 (2004).

E. Santiso and K.E. Gubbins, "Multi-Scale Molecular Modeling of Chemical Reactivity", *Molecular Simulation*, **30**, 699-748 (2004) [invited review paper]

T.J. Bandoz, M.J. Biggs, K.E. Gubbins, Y. Hattori, T. Iiyama, K. Kaneko, J. Pikunic and K. Thomson, "Molecular Models of Porous Carbons", *Chemistry and Physics of Carbon*, **28**, 41-228 (2003).

F.R. Siperstein and K.E. Gubbins, "Phase Separation and Liquid Crystal Self-Assembly in Surfactant-Inorganic-Solvent Systems", *Langmuir*, **19**, 2049-2057 (2003).

C.M. Colina, C.G. Olivera-Fuentes, F.R. Siperstein, M. Lísal and K.E. Gubbins, "Thermal Properties of Supercritical Carbon Dioxide by Monte Carlo Simulations", *Molecular Simulation*, **29**, 405-412 (2003).

F.R. Hung, K.E. Gubbins, R. Radhakrishnan, F. Beguin and M. Sliwinska-Bartkowiak, "Freezing/Melting in Porous Carbons", *Proceedings of the 3<sup>rd</sup> Pacific Basin Conference on Adsorption Science and Technology*, ed. C-H. Lee, World Scientific, Singapore, pp. 9-16 (2003).

Colina, C. M. and K.E. Gubbins, "Choosing and Evaluating Equations of State for Thermophysical Properties", *Chemical Engineering Education*, **37**, 236-240 (2003).

J. Pikunic and K.E. Gubbins, "Molecular Dynamics Simulations of Simple Fluids Confined in Realistic Models of Nanoporous Carbons", *European Physical Journal*, **12**, 35-40 (2003).

C.H. Turner and K.E. Gubbins, "Effects of Supercritical Clustering and Selective Confinement on Reaction Equilibrium: A Molecular Simulation Study of the Esterification Reaction", *Journal of Chemical Physics*, **119**, 6057-6067 (2003).

C.M. Colina, T.A. Walker, R.J. Spontak and K.E. Gubbins, "The Influence of High-Pressure Carbon Dioxide on the Phase Behavior of PDMS/PEMS Blends: An Experimental and Theoretical Investigation", *Proc. 6<sup>th</sup> International Symp. on Supercritical Fluids*, Versailles, April 2003.

Striolo, A.A. Chialvo, P.T. Cummings and K.E. Gubbins, "Water Adsorption in Carbon-Slit Nanopores", *Langmuir*, **19**, 8583-8591 (2003).

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

J. Pikunic, C. Clinard, N. Cohaut, K.E. Gubbins, J.-M. Guet, R.J. Pellenq, I. Rannou and J.-N. Rouzaud, "Structural Modeling of Porous Carbons: Constrained Reverse Monte Carlo Method", *Langmuir*, **19**, 8565-8582 (2003).

M. Lisal, C.K. Hall, K.E. Gubbins and A.Z. Panagiotopoulos, "Formation of Spherical Micelles in a Supercritical Solvent: Lattice Monte Carlo Simulation and Multicomponent Solution Model", *Molecular Simulation*, **29**, 139-157 (2003).

J. Pikunic, K.E. Gubbins, R.J.-M. Pellenq, N. Cohaut, I. Rannou, J.-M. Guet, C. Clinard and J.-N. Rouzaud, "Realistic Molecular Models for Saccharose-Based Carbons", *Applied Surface Science*, **196**, 98-104 (2002).

C.M. Colina, M. Lisal, F.R. Siperstein and K.E. Gubbins, "Accurate CO<sub>2</sub> Joule-Thomson Inversion Curve by Molecular Simulations", *Fluid Phase Equilibria*, **202**, 253 (2002).

F.R. Siperstein and K.E. Gubbins, "Influence of Synthesis Conditions on Surface Heterogeneity of M41 Type Materials Studied with Lattice Monte Carlo", in "Characterization of Porous Solids VI", Studies in Surface Science and Catalysis Vol. 144, eds. F. Rodriguez-Reinoso, B. McEnaney, J. Rouquerol and K. Unger, pp. 647-654, Elsevier, Amsterdam (2002).

J. Pikunic, C. Clinard, N. Cohaut, K.E. Gubbins, J.-M. Guet, R.J.-M. Pellenq, I. Rannou and J.-N. Rouzaud, "Reconstruction Method for the Characterization of Porous Carbons", in "Characterization of Porous Solids VI", Studies in Surface Science and Catalysis Vol. 144, eds. F. Rodriguez-Reinoso, B. McEnaney, J. Rouquerol and K. Unger, pp. 19-26, Elsevier, Amsterdam (2002).

M. Sliwinska-Bartkowiak, G. Dudziak, R. Radhakrishnan and K.E. Gubbins, "Freezing in Mesopores: Aniline in Silica Glasses and MCM-41", in "Characterization of Porous Solids VI", Studies in Surface Science and Catalysis Vol. 144, eds. F. Rodriguez-Reinoso, B. McEnaney, J. Rouquerol and K. Unger, pp. 467-474, Elsevier, Amsterdam (2002).

J. Pikunic, C.M. Lastoskie and K.E. Gubbins, "Molecular Modeling of Adsorption from the Gas Phase", in *Handbook of Porous Solids*, Ch. 2.5.1, eds. F. Schüth, K.S.W. Sing and J. Weitkamp, pp. 182-236, Wiley-VCH, Weinheim (2002).

R. Radhakrishnan, K.E. Gubbins and M. Sliwinska-Bartkowiak, "Existence of a Hexatic Phase in Confined Systems", *Physical Review Letters*, **89**, 076101 (2002).

C.H. Turner, J.K. Brennan, J.K. Johnson and K.E. Gubbins, "Effect of Confinement by Porous Materials on Chemical Reaction Kinetics", *Journal of Chemical Physics*, **116**, 2138-2148 (2002).

C.H. Turner, J.K. Brennan, J. Pikunic and K.E. Gubbins, "Simulation of Chemical Reaction Equilibria and Kinetics in Heterogeneous Carbon Micropores", *Applied Surface Science*, **196**, 366-374 (2002).

M. Lisal, C.K. Hall, K.E. Gubbins and A.Z. Panagiotopoulos, "Self-Assembly of Surfactants in a Supercritical Solvent from Lattice Monte Carlo Simulations", *J. Chem. Phys.*, **116**, 1171-1184 (2002).

John K. Brennan, Kendall T. Thomson and Keith E. Gubbins, "Water in Porous Carbons: A Simulation Study", *Fundamentals of Adsorption 7*, eds. K. Kaneko, H. Kanoh and Y. Hanzawa, International Adsorption Society (IK International Pub.), p. 426 (2002).

John K. Brennan, Kendall T. Thomson and Keith E. Gubbins, "Adsorption of Water in Activated Carbons: Effects of Pore Blocking and Connectivity", *Langmuir*, **18**, 5438-5447 (2002).

M. Lisal, C.K. Hall, K.E. Gubbins and A.Z. Panagiotopoulos, "Micellar Behavior in Supercritical Solvent-Surfactant Systems from Lattice Monte Carlo Simulations", *Fluid Phase Equilibria*, **194-197**, 233-247 (2002).

C.H. Turner and K.E. Gubbins, "Chemical Reaction Equilibria in Carbon Micropores from Monte Carlo Simulation:  $2\text{NO} = (\text{NO})_2$  and  $\text{N}_2 + 3\text{H}_2 = 2\text{NH}_3$ ", *Fundamentals of Adsorption 7*, eds. K. Kaneko, H. Kanoh and Y. Hanzawa, International Adsorption Society (IK International Pub.), p. 489 (2002).

S. Gavaldà, K.E. Gubbins, Y. Hanzawa, K. Kaneko and K.T. Thomson, "Nitrogen Adsorption in Carbon Aerogels: A Molecular Simulation Study", *Langmuir*, **18**, 2141-2151 (2002).

R. Radhakrishnan, K.E. Gubbins and M. Sliwinska-Bartkowiak, "Global Phase Diagrams for Freezing in Porous Media", *Journal of Chemical Physics*, **116**, 1147-1155 (2002).

C.M. Colina, C.K. Hall and K.E. Gubbins, "Phase Behavior of PVAC-PTAN Block Copolymer in Supercritical Carbon Dioxide Using SAFT", *Fluid Phase Equilibria*, **194-197**, 553-565 (2002).

C.M. Colina, L.F. Turrens, C. Olivera-Fuentes, K.E. Gubbins and L.F. Vega, "Prediction of the Joule-Thomson Inversion Curve for the n-Alkane Series and Carbon Dioxide from the Soft-SAFT Equation of State", *Industrial Engineering Chemistry Research*, **41**, 1069-1075 (2002).

Christian M. Lastoskie and Keith E. Gubbins, "Characterization of Porous Materials Using Molecular Theory and Simulation", in "Molecular Modeling and Theory in Chemical Engineering", ed. A. Chakraborty, *Advances in Chemical Engineering*, **28**, 203-250 (2001). [Invited review paper]

E.A. Müller and K.E. Gubbins, "Molecular-Based Equations of State for Associating Fluids: A Review of SAFT and Related Approaches", *Industrial & Engineering Chemistry Research*, **40**, 2193-2211 (2001).

J. Pikunic, R.J.-M. Pellenq, K.T. Thomson, J.-N. Rouzaud, P. Levitz and K.E. Gubbins, "Improved Molecular Models for Porous Carbons", *Studies in Surface Science & Catalysis*, **132**, 647-652 (2001).

M. Sliwinska-Bartkowiak, G. Dudziak, R. Sikorski, R. Gras, K.E. Gubbins, R. Radhakrishnan and K. Kaneko, "Freezing Behavior in Porous Materials: Theory and Experiment", *Polish Journal of Chemistry*, **75**, 547-555 (2001).

M. Sliwinska-Bartkowiak, G. Dudziak, R. Sikorski, R. Gras, K.E. Gubbins and R. Radhakrishnan, "Dielectric Studies of Freezing Behavior in Porous Materials: Water and Methanol in Activated Carbon Fibers", *Phys. Chem. Chem. Phys.*, **3**, 1179-1184 (2001).

M. Sliwinska-Bartkowiak, G. Dudziak, R. Gras, R. Sikorski, R. Radhakrishnan, and K.E. Gubbins, "Freezing Behavior in Porous Glasses and MCM-41", *Colloids & Surfaces A*, **187-188**, 523-529 (2001).

J. Brennan, T.J. Bandosz, K.T. Thomson and K.E. Gubbins, "Water in Porous Carbons", *Colloids & Surfaces A*, **187-188**, 539-568 (2001).

S. Gavaldà, K. Kaneko, K.T. Thomson and K.E. Gubbins, "Molecular Modeling of Carbon Aerogels", *Colloids & Surfaces A*, **187-188**, 531-538 (2001).

M. Sliwinska-Bartkowiak, G. Dudziak, R. Sikorski, R. Gras, R. Radhakrishnan and K.E. Gubbins, "Melting/Freezing Behavior of a Fluid Confined in Porous Glasses and MCM-41: Dielectric Spectroscopy and Molecular Simulation", *Journal of Chemical Physics*, **114**, 950-962 (2001).

C.H. Turner, J.K. Johnson and K.E. Gubbins, "Effect of Confinement on Chemical Reaction Equilibria: The Reactions  $2\text{NO} = (\text{NO})_2$  and  $\text{N}_2 + 3\text{H}_2 = 2\text{NH}_3$  in Carbon Micropores", *Journal of Chemical Physics*, **114**, 1851-1859 (2001).

K.P. Travis and K.E. Gubbins, "Computer Simulation of Isothermal Mass Transport in Graphitic Slit Pores", *Molecular Simulation*, **27**, 405-439 (2001).

C.H. Turner, J. Pikunic and K.E. Gubbins, "Influence of Chemical and Physical Surface Heterogeneity on Chemical Reaction Equilibria in Carbon Micropores", *Molecular Physics*, **99**, 1991-2001 (2001).

F.R. Siperstein and K.E. Gubbins, "Synthesis and Characterization of Templated Mesoporous Materials using Molecular Simulation", *Molecular Simulation*, **27**, 339-352 (2001).

M. Sliwinska-Bartkowiak, R. Radhakrishnan and K.E. Gubbins, "Effect of Confinement on Melting in Slit-Shaped Pores: Experimental and Simulation Study of Aniline in Activated Carbon Fibers", *Molecular Simulation*, **27**, 323-3337 (2001).

E.A. Müller and K.E. Gubbins, "Associating Fluids and Fluid Mixtures", in *Equations of State for Fluids and Mixtures*, edited by J.V. Sengers, R.F. Kayser, C.J. Peters and H.J. White, Jr., Elsevier, Amsterdam, pp 435-478 (2000).  
[Invited review paper]

A.V. Shevade, S. Jiang and K.E. Gubbins, "Molecular Simulation of Water-Methanol Mixtures in Activated Carbon Pores: A Molecular Simulation Study", *Journal of Chemical Physics*, **113**, 6933-6942 (2000).

K.P. Travis and K.E. Gubbins, "Combined Diffusive and Viscous Transport of Methane in a Carbon Slit Pore", *Molecular Simulation*, **25**, 209-227 (2000).

K. T. Thomson and K.E. Gubbins, "Modeling Structural Morphology of Porous Carbons by Reverse Monte Carlo", *Langmuir*, **16**, 5761-5774 (2000).

E.A. Müller, F.R. Hung and K.E. Gubbins, "Adsorption of Water Vapor-Methane Mixtures on Activated Carbons", *Langmuir*, **16**, 5418-5424 (2000).

M. Miyahara, H. Kanda, K. Higashitani and K.E. Gubbins, "Molecular Simulation Study on Freezing in Nano-Pores", *Characterization of Porous Solids V*, ed. K.K. Unger, G. Kreysa and J.P. Baselt, Elsevier, Amsterdam, pp. 31-40 (2000).

C.M. Lastoskie and K.E. Gubbins, "Characterisation of Porous Materials using Density Functional Theory and Molecular Simulation", *Characterization of Porous Solids V*, ed. K.K. Unger, G. Kreysa and J.P. Baselt, Elsevier, Amsterdam, pp. 41-50 (2000). [Invited review paper]

L.D. Gelb and K.E. Gubbins, "Characterisation of Porous Glasses: Molecular Simulation of Adsorption", *Characterization of Porous Solids V*, ed. K.K. Unger, G. Kreysa and J.P. Baselt, Elsevier, Amsterdam, pp. 61-69 (2000).

M. Sliwinska-Bartkowiak, J. Gras, R. Sikorski, G. Dudziak, R. Radhakrishnan and K.E. Gubbins, "Experimental and Simulation Studies of Melting and Freezing in Porous Glasses", *Characterization of Porous Solids V*, ed. K.K. Unger, G. Kreysa and J.P. Baselt, Elsevier, Amsterdam, pp. 141-150 (2000).

R. Radhakrishnan, K.E. Gubbins, M. Sliwinska-Bartkowiak and K. Kaneko, "Understanding Freezing Behavior in Pores", *Adsorption Science and Technology*, ed. D.D. Do, World Scientific, Singapore, pp. 234-238 (2000).

K.T. Thomson, J. Pikunic and K.E. Gubbins, "An Improved Model of Microporous Carbon Morphology Using Molecular Simulation", *Adsorption Science and Technology*, ed. D.D. Do, World Scientific, Singapore, pp. 239-243 (2000).

C.H. Turner, J. Brennan, K.E. Gubbins and J.K. Johnson, "Effect of Confinement on Chemical Reaction Equilibrium", *Adsorption Science and Technology*, ed. D.D. Do, World Scientific, Singapore, pp. 244-248 (2000).

R. Radhakrishnan, K.E. Gubbins and M. Sliwinska-Bartkowiak, "Effect of the Fluid-Wall Interaction on Freezing of Confined Fluids: Towards the Development of a Global Phase Diagram", *Journal of Chemical Physics*, **112**, 11048-11057 (2000).

John K. Brennan, Kendall T. Thomson and Keith E. Gubbins, "Simulation of Water in Porous Carbons", Proceedings of the Foundations of Molecular Modeling and Simulation (FOMMS) Conference, Keystone, CO (2000).