Diffusion Fundamentals I

Basic Principles of Theory, Experiment and Application

September 21st - 24th, 2005 – Leipzig, Germany

POSTER PRESENTATIONS

Poster Presentation I, Thursday, September 22nd 14.00 – 15.00

Fluids

1 Residue Specific Studies of NH Exchange Rates Performed on Ubiquitin
T. Brand, G. A. Morris, E. J. Cabrita, H.-J. Hofmann, S. Berger

2 Diffusion Exchange NMR Spectroscopic Study of Dextran Exchange through Polyelectrolyte Multilayer Capsules
P. Galvosas, Y. Qiao, T. Adalsteinsson, M. Schönhoff, P. T. Callaghan

3 Theory and Simulation of Fick's Historical Verification of the 2nd Law
M. E. Glicksman, R. DiDomizio, A. Lupulescu

4 Molecular Motions of Calix[4]Arene and Thiacalix[4]Arene in Solution Studied by NMR Relaxation
J. Lang, K. Šetková, V. Deckerová, P. Lhoták, J. Czernek

5 Particle Diffusion Coefficient and Dynamic Viscosity in Non-Ideal Liquid Mixtures by Dynamic Light Scattering
C. Botero, H. Kremer, A. P. Fröba, A. Leipertz

6 Liquid Viscosity and Surface Tension by Surface Light Scattering
A. P. Fröba, C. Botero, H. Kremer, A. Leipertz

7 Mutual Diffusion Coefficient in Fluids by Dynamic Light Scattering
A. P. Fröba, C. Botero, H. Kremer, A. Leipertz

8 Thermal Diffusivity of Fluids by Dynamic Light Scattering
H. Kremer, C. Botero, A. P. Fröba, A. Leipertz

9 NMR Diffusion Experiments for Complex Systems
K. I. Momot, D. G. Regan, P. W. Kuchel

10 Molecular Motion in Thin Liquid Films near Surface Steps
A. Schob, F. Cichos

11 Self-Diffusion Slowdown in Liquid Indium and Gallium under Confinement
P. Sedykh, E. V. Charnaya, Cheng Tien, D. Michel, M.K. Lee, W. Wang

12 Multicomponent Diffusion Coefficients in Liquids from Model-Based Raman Spectroscopy
A. Bardow, V. Göke, H.-J. Koß, E. Kriesten, K. Lucas, W. Marquardt

13 Apparent Longitudinal Relaxation of Mobile Spins in Thin, Periodically Excited Slices
A. Gädke, N. Nestle

Theory and Modelling (part I)

Poster Presentation II, Friday, September 23rd 14.00 – 16.00

Theory and Modelling (part II)

21 Molecular Traffic Control in Porous Nanoparticles
A. Brzank, G. Schütz

22 Anomalous Knudsen Diffusion in Simple Pore Models
A.J. Dammers, M.-O. Coppens

23 Potential Calculations and MD Simulations of *n*-Pentane in Silicalite-1
A. Loisruangsin, S. Fritzsche, S. Hannongbua

24 Exploring the Extreme Transport Conditions through Membranes by Molecular Dynamics Simulations
J. Gulín-González, A. Schüring, S. Vasenkov, S. Fritzsche, J. Kärger

25 Rotational Motion of n-Pentane in H-ZK5
O. Saengsawang, P. C. M. M. Magusin, T. Remsungnen, A. Loisruangsin, S. Fritzsche, A. Schüring, S. Hannongbua

26 Entropic Barriers for the Diffusion of Molecules under Confinement
A. Schüring, S. Fritzsche, S. M. Auerbach

27 Molecular Simulation of Gas Transport in Nanoporous Carbons
Qiong Cai, A. Buts, N. Seaton, M. Biggs

28 Diffusion between Interstitial Sites in the Hexagonal C14 AB_2 Structure
C. A. Sholl

29 Numerical Evidence for the Validity of the Local Equilibrium Hypothesis - The n-Octane Vapor-Liquid Interface
J.-M. Simon, S. Kjelstrup, D. Bedeaux

30 Kinetics of Adsorption of Linear and Branched C6 Alkanes onto ZSM-5 Zeolite - Experiments and Molecular Simulations
J.-M. Simon, E. Fardet-Lemaire, I. Bezverkhyy, J.-P. Bellat, F. Baras

31 Determining Binary Diffusion Coefficients for Mixtures in Zeolites from PFG NMR, MD Simulation, and Theory
Qi Zhao, Shaji Chempath, R. Q. Snurr

32 A CTRW Interpretation of Simulated Single-file Diffusion in Zeolites
P. Demontis, G. B. Suffritti

33 A "Coarse-grained" Model based on a Cellular Automaton for the Study of Diffusion in Microporous Materials
P. Demontis, F. G. Pazzona, G. B. Suffritti

34 Effects of Surface Roughness on Transport Properties of Porous Media
M. Kainourgiakis, T. Steriotis, E. Kikkinides, A. Stubos, S. Vasenkov

35 Self- and Transport Diffusion in Narrow Pores with Different Roughness
S. Zschiegner, S. Russ, A. Bunde, J. Kärger

36 Understanding the Loading Dependence of Self-Diffusion in Carbon Nanotubes
S. Jakobtorweihen, C. P. Lowe, F. J. Keil, B. Smit

37 A Molecular Dynamics study of the diffusion coefficients in water-tertbutyl alcohol mixtures: A comparison between All-Atoms and United-Atoms models.
F.H.R Leroy, A.D. Mackie, P. Miró, C. Bo and J. Bonet Avalos

38 Self-diffusion of *n*-alkanes in MFI-type zeolites: A Molecular Dynamics study and a comparison to Quasi-Elastic Neutron Scattering experiments.
F.H.R Leroy, H. Jobic, B. Rousseau and A.H. Fuchs

39 Anomalous Diffusion in Ionically Conducting Glasses
J. Habasaki, K. L. Ngai, Y. Hiwatari

40 Modelling of Diffusion-Controlled Pattern Formation in Thin Metallic Film Growth on Crystalline Substrates
V. Kuzovkov, E. Kotomin, G. Zvejnieks

41 Calculation of the Effective Diffusion Coefficient for Heterogeneous Media
J.R. Kalnin, E.A. Kotomin, J. Maier, V.N. Kuzovkov

42 Molecular Dynamic Simulation on Adsorption of Chlorinated Hydrocarbon into High-Silica Zeolite
K. Chihara, H. Minaki, T. Sasaki

43 Theory of Diffusion under Stress
A. V. Nazarov, A. A. Mikheev

44 N-Body Potentials in Simulation of Point Defect Properties
A. S. Chirkov, A. V. Nazarov

45 Stimuli and Mechanisms of Diffusion Mass-Transport in the Processes of Structural-Phase Changes in Metallic Materials under High-Rate Deformation
Y.S. Nechaev

46 Mechanisms of Hydrogen Sorption, Solubility and Diffusivity in Carbon Nanomaterials, Relevance to the On-Board Storage Problem
Y.S. Nechaev

47 On the Physics of the Apparent Solubility and Diffusivity of Hydrogen in Metals and Alloys, Relevance for Revealing the Hydrogen-Assisted Damage Micromechanisms
Y.S. Nechaev

48 Anomalies of the Diffusion Mass-Transfer during 2D-Decomposition of Superconducting $Yba_2Cu_3O_{6+X}/Y_2BaCuO_5$ Composites
Y.S. Nechaev

49 Calculation of Diffusivities in Ordering f.c.c. Alloy by the Kinetic Data about Short- and Long-Range Order Parameters' Relaxation
T. Radchenko, V. Tatarenko, S. Bokoch

50 Boundary-Value Problems for the Diffusion Equation in Domains with Disconnected Boundary
S. D. Traytak

51 Simulation of Diffusion under Pressure in BCC Metals
I. Valikova, A. Nazarov

52 Oxygen Transport and Association in Yttria Stabilised Zirconia
M. Kilo, R. A. Jackson

53 Modelling of Anion Transport in YZrON
M. Kilo, T. Bredow

54 Diffusion of Methanol in Zeolites: a Molecular Dynamics Study
D. F. Plant, G. Maurin, R. G. Bell

Solids

55 Computer Simulation of the Formation of Hollow Nanocrystals
I. V. Belova, G. E. Murch

56 Carbon Interstitial Diffusion in γ-Fe
I. V. Belova, G. E. Murch

57 A Microscopic Flow Model Based on Brownian Dynamics for Simulating Ionic Diffusion in Glasses
G. Darricarrere, J. Dutour, F. Henn

58 Surface Diffusion and Growth of Alloy Nanoclusters: A Monte Carlo Study
S. Heinrichs, M. Einax, W. Dieterich, P. Maass, A. Majhofer

59 Numerical Study of Grain Boundary Diffusion: Size Effects
D. Gryaznov, J. Fleig, J. Maier

60 Li Diffusion in $LiAlO_2$ Single Crystals Studied with NMR Spectroscopy
S. Indris, R. Uecker, P. Heitjans

61 $BaTiO_3$ Formation by Solid State Reactions on Rutile Single Crystals
A. Lotnyk, S. Senz, D. Hesse

62 Proton Diffusion and Mobility in Condensed Matter
K. D. Kreuer

63 Diffusion of Nano-Sized Liquid Pb Inclusions in Thin Aluminum Foils
S. Prokofjev, V. Zhilin, E. Johnson, U. Dahmen

64 A Theoretical Model of Interaction between Titanium and Binary Rarified Gas Media with Taking into Account the Segregation of Impurities on the Interface and in the Bulk of the Metal
Ya. Matychak, A. Prytula, V. Fedirko, I. Pohreljuk

65 Dynamics in FePt Thin Films Studied by Grazing Incidence Synchrotron Reflexion on Isotopic Multilayers
M. Rennhofer, M. Sladecek, D. Kmiec, S. Stankov, B. Sepiol, G. Vogl, R. Rüffer, A. Vantomme, J. Meersschaut

66 Fundamentals of Self-Diffusion in Amorphous Si-(B-)C-N
H. Schmidt

67 Enhanced Ionic Conductivity in Heavily Doped Ceria Nanoceramics
M. G. Bellino, D. G. Lamas, N. E. Walsöe de Reca

68 Ultraslow Cation Diffusion in Li Intercalated Cubic TiS_2
M. Wilkening, P. Heitjans

69 Interdiffusion in Quasi-Ternary Semiconductor Systems of GeTe/SnTe/PbTe
L. V. Yashina, V. Leute, H. M. Schmidtke, V. I. Shtanov

70 Formation Mechanism of Plateau, Rapid Fall and Tail in Phosphorus Diffusion Profile in Silicon Based on the Pair Diffusion Models of Vacancy Mechanism and Interstitial Mechanism
Masayuki Yoshida, Masami Morooka, Shuji Tanaka, Manabu Takahashi

Soft Matter: From (Bio-)Molecules to Man

71 Spatial Redistribution of Boron Implanted into Poly-(Di-n-Hexyl Silane), (PDHSi)
D. Fink, M. Müller, M. Behar, R. M. Papaleo

72 Entropic Forces Generated by Grafted Semi-flexible Polymers
A. Gholami, J. Wilhelm, Erwin Frey

73 Probing Pore-Structure within Porous Polymer Particles by NMR
E. W. Hansen, H. C. Gran

74 Ultraslow Molecular Dynamics of Organized Fluids: NMR Experiments and Monte-Carlo Simulations
F. Grinberg

75 Drug penetration studied by FTIR methods
B. D. Hanh, U. Günther, M. Hartmann, S. Wartewig, R. Neubert

76 Fast Optical Tracking of Diffusion in Brain Extracellular Space
J. Hrabe, S. Hrabetova

77 Dead Spaces Hinder Diffusion and Contribute to Tortuosity of Brain Extracellular Space
S. Hrabetova, Lian Tao, J. Hrabe, C. Nicholson

78 Modelling Aroma Release from Silica Sol-Gel Particles Using Self-Diffusion Data Obtained Under Magic Angle Spinning Conditions
S. R. Veith, F. M. Berruex, E. Hughes, S. E. Pratsinis

79 Fluid Self-Diffusion in Scots Pine Sapwood and Silica Wood Replicas
E. H. Johannessen, E. W. Hansen, J. B. Rosenholm

80 How to Measure Subdiffusion Coefficient
T. Kosztolowicz

81 Computer Simulation - Influence of Corset Effect
M. Kroutieva, T. Shakirov, N. Fatkullin, R. Kimmich

82 Subdiffusive Reaction Front in the Enamel Caries Process
T. Kosztolowicz, K. D. Lewandowska

83 Studies on Diffusion of Rhodamine B Labeled Polystyrene in Dilute and Semidilute Solutions by Fluorescence Correlation Spectroscopy
Ruigang Liu, W. Oppermann

84 Lateral Diffusion of Proteins in Cell Membrane: The Anomalous Case
A. Lubelski, J. Klafter

85 Uptake of the Herbicide 2,4-Dichlorophenoxyacetate (2,4-D) by *Delftia acidovorans* MC1 - Complex Kinetic Characteristics in Dependence of pH and Growth Substrate
R. H. Müller, D. Hoffmann

86 Measurement of Local Diffusion Properties in Brain Tissue
C. Nicholson, Lian Tao, S. Hrabetova, R. G. Thorne

87 ESRI Study of Diffusion Processes in Poly(2-Hydroxyethyl Methacrylate) Gels and Concentrated Solutions
A. Marek, J. Labský, J. Pilař

88 Diffusivity of Water in a Biological Model Membrane: an NMR Study
M. Rudakova, A. Filippov

89 Water Diffusion through Asymmetric Polymer Membranes and Polyelectrolyte Multilayers
A. Sagidullin, J. Meier-Haack, U. Scheler

90 Study of diffusion coefficient of water and homologous series of primary alcohols in PEBA membranes by NMR
N. Scharnagl, Norbert Stribeck, Veroni Barbi

91 Comparing the Biophysical Properties of Sterols in Lipid Membranes – What is Special about Cholesterol?
H. A. Scheidt, P. Müller, A. Herrmann, K. Arnold, K. Gawrisch, D. Huster

92 Varying the Gradient Pulse Length Gives Valuable Information in NMR Diffusometry
O. Söderman, D. Topgaard

93 Ultra fast processes for solvent evaporation in thin polymer films below T_g
M. Souche, D. Long

94 Effects of Ion Pairs on Mass and Charge Transport in a Crosslinked Amorphous Polymer Electrolyte
S. Obeidi, S.J. Pas, N.A. Stolwijk

95 PFG NMR Studies of Diffusion in Sulfonic Acid Based Systems
A. Telfah, G. Majer

96 MRI Study of Fickian, Case II and Anomalous Diffusion of Solvents into HPMC
J. Tritt – Goc, J. Kowalczuk

97 Pulsed Field Gradient NMR in Combination with Magic Angle Spinning - New Possibilities for Studying Diffusion in Lipid Membranes and Heterogeneous Materials
A. Pampel

98 Influence of Phase Transitions on the Mobility of Organic Pollutants in Synthetic and Natural Polymers
U. Roland, K. W. Fomba, F. Stallmach, P. Galvosas, J. Kärger, F.-D.-Kopinke

99 Anisotropic Solute and Solvent Diffusion in Protein Crystals
R. Archipov, A. Cvetkovic, F. Stallmach, A. J.J. Straathof

100 Influence of Domains on Lateral Diffusion in Lipid Bilayers: PFG NMR Study
S. Vasenkov, K. Ulrich, C. Selle, J. Kärger, J. Käs

101 Emulsion Droplet Size Distribution by PFG NMR: High Concentrations, Small Radii, and Suspo-Emulsions
Jianqin Zhuang, R. Voelkel

102 Ionic Aggregation of Metallocene Olefin Polymerization Catalysts: A PFG NMR Study
B. Endeward, P. Brant, M. Bernardo, H. Thomann

103 Lattice and Grain Boundary Diffusion of Cations in Tetragonal Zirconia
S. Swaroop, M. Kilo, Ch. Argirusis, G. Borchardt, A. H. Chokshi

104 Monte Carlo Study of Transport Phenomena in Surface Binary Alloys
A. De Virgiliis, K. Binder

105 Static and dynamic properties of absorbed water in Chabazite: A molecular dynamics study
S. Jost, P. Biswas, S. Fritzsche, A. Schüring, J. Kärger, R. Heberlandt

Poster Presentation III, Saturday, September 24th 08.30 – 09.30

Holes and Channels

110 Diffusion of Cyclohexane and Cyclopentane Confined in Mesoporous MCM-41
D. W. Aksnes, K. Førland

111 Evidence for Subdomains in Large Crystals of NaX Zeolite
Z. Adem, F. Guenneau, M.-A. Springuel-Huet, A. Gédéon

112 From "Fast" to "Slow" Liquid-vapor Exchange in Partially Filled Porous Media. A Field-gradient NMR Diffusometry Study
I. Ardelean, G. Farrher, C. Mattea, R. Kimmich

113 Synthesis and Catalytic Performance of Large Zeolite Y Crystals
C. Berger, R. A. Rakoczy, R. Gläser, J. Weitkamp

114 Diffusion of n-Alkanes in MFI-Type Zeolites: a Comparative Study with Different Measuring Techniques
V. Bourdin, S. Brandani, A. Gunadi, H. Jobic, C. Krause, J. Kärger, W. Schmidt

115 Effect of Water Adsorption on the Thermodynamics and Dynamics of the Extra-Framework Cations in Zeolite Systems
B. Coasne, G. Maurin, A. Nicolas, S. Devautour-Vinot, J.-C. Giuntini, F. Henn

116 Molecular Transport in Inorganic Membranes: CO_2 / CH_4 Separation
E. W. Corcoran

117 Moments Method Applied to the In-Situ Characterisation of Normal Butane Mass Transfer in MFI Zeolite Membranes
L. Courthial, A. Baudot, E. Jolimaitre, M. Tayakout, C. Jallut

118 Coefficients in Solid-State Diffusion by Inverse Gas Chromatography
A. V. Dremetsika, P. A. Siskos, N. A. Katsanos

119 Effect of the Acid Properties on the Diffusion of C_7 Hydrocarbons in UL-ZSM-5 Materials
Hoang Vinh-Thang, Qinglin Huang, A. Ungureanu, M. Eić, Do Trong-On, S. Kaliaguine

120 Transport Properties of Catalyst Supports Derived from a Catalytic Test Reaction
F. Friedel, F. Janowski, T. Hahn, D. Enke

121 Time dependent diffusion studies in partially filled porous glasses using the MAGROFI technique
German Farrher, Ioan Ardelean, Rainer Kimmich

122 NMR Imaging as a Tool for Studying the Diffusion and Co-Diffusion of Gases in Zeolite Catalysts
J. Fraissard

123 Diffusion in Multicomponent Gas Adsorption on MSC5A, Chromatographic Study
Kazuyuki Chihara, Yosuke Kaneko, Takuya Terakado, Hisashi Mizuochi

124 Single Molecule Spectroscopy: Translational and Rotational Diffusion of Single Fluorescent Dyes in Nano-Structured Porous Materials
J. Kirstein, C. Jung, C. Hellriegel, C. Bräuchle

125 Mass Transport in the Hierarchical Porous Structure of Zeolite-Based Composite Membranes
A. Zikánová, P. Hrabánek, M. Kočiřík, L. Brabec, K. Juristová, P. Čapek, B. Bernauer, V. Hejtmánek, O. Šolcová, P. Uchytil

126 Concentration Dependence of Transport and Corrected Diffusivities of n-Hexane in Silicalite Measured by QENS
N. Laloué, C. Laroche, H. Jobic

127 Azeotropic Adsorption of Organic Solvent Vapor Mixture on High Silica Zeolite, Mass Transfer Dynamics
Kazuyuki Chihara, Takashi Matsumoto, Kazunori Hijikata

128 The Release Properties of the Mesoporous Materials SBA-15 and PHTS for their Use in the Controlled Release of Ibuprofen and Vancomycin
K. J.F. Lievens, V. Meynen, P. Cool, E. F. Vansant, G. V. Baron, J. F.M. Denayer

129 The Sorption Dynamics of C_3 Hydrocarbons over Carbon Nanotubes
G. Onyestyák, Z. Ötvös, J. Valyon, I. Kiricsi, L. V. C. Rees

130 The working range of static field gradient NMR illustrated by measurements of the intracrystalline diffusion of water in NaA-zeolites
H. Pahlke, B. Geil, D. Kruk, F. Fujara

131 Measurement of Diffusivities of Helium and Argon in Silicalite by Static Single Crystal Membrane Technique
E. Chalhoub, D.B. Shah

132 Diffusion of BTX in MSC5A in Supercritical CO_2
Kazuyuki Chihara, Ryota Suzuki, Naoki Omi

133 Gas Diffusion in Polycrystalline MFI-Type Zeolite Membranes
Hiromitsu Takaba, Atsushi Yamamoto, Kikuko Hayamizu, Shin-ichi Nakao

134 Adsorption and Self-Diffusion of Water and Benzene Molecules Adsorbed in Synthetic Opal Samples
R. Vartapetian, E. Khozina, I. Bardyshev

135 Synthesis and Characterization of Carbon Nanotube Arrays
E. Vermisoglou, G. Pilatos, V. Georgakilas, E. Topoglidis, N. Kanellopoulos

136 Innovative Methods for the Characterization of Ceramic Nanofiltration Membranes Modified by TEOS/O3 Chemical Vapor Deposition
G.E. Romanos, A. Labropoulos, N. Kanellopoulos

137 Effect of carbonization process on the structure and the gas permeation properties of polyimide hollow fiber membranes.
E. P. Favvas, G. C. Kapantaidakis and N. K. Kanellopoulos

138 Transport Diffusivity in Zeolites: Possible Reasons for Misleading Results of Macroscopic Techniques
C. Chmelik, P. Kortunov, S. Vasenkov, T. Ito, J. Kärger, J. Konatowski, J. Weitkamp, D. M. Ruthven

139 New Options for Measuring Molecular Diffusion in Zeolites by MAS PFG NMR
M. Fernandez, A. Pampel, D. Freude, J. Kärger

140 PFG NMR Measurement of Molecular Diffusion in Cation-Free Zeolites of Type LTA
A. Corma, J. Kärger, C. Krause

141 A Remarkable Non-Monotonical Chain-Length Dependence: Diffusion of n-Alkanes in Zeolites LTA
S. Brandani, J. Caro, H. Jobic, C. Krause, J. Kärger, A. Möller, D. M. Ruthven, R. Staudt, Xiaobo Yang

142 Separation Based on Molecular Level Using Zeolitic Membranes
S. Khajavi, F. Kapteijn, J.C. Jansen

143 Transport Properties of Guest Molecules in Mesoporous SBA-15 Materials - A PFG NMR Study
P. Kortunov, R. Valiullin, J. Kärger, V. Meynen, E. Vansant

144 Time- and Spatially-Resolved Study of Methanol Sorption in Ferrierite Crystals using Interference and IR Microscopy
P. Kortunov, C. Chmelik, J. Kärger, R. A. Rakoczy, D. M. Ruthven, Y. Traa, S. Vasenkov, J. Weitkamp, T. Ito

145 NMR Studies of Diffusion and Pore Size Distribution on Water-Containing Aquifer Rocks and Construction Materials
W. Schönfelder, F. Stallmach, H. Huinink, K. Kopinga

146 Analytical Model for Extrapolation of Experimental NMR Diffusion Studies to Reaction Conditions for Formulated Catalyst Particles
F. Stallmach, S. Crone

147 Adsorption Hysteresis in Nanopores: Options to a Comparative Study Using Nuclear Magnetic Resonance and Computer Simulation Methods
R. Valiullin, J. Kärger, P. Monson

148 Investigations of Molecular Diffusion in FCC Catalysts
P. Kortunov, S. Vasenkov, J. Kärger, M. Fé Elía, M. Perez, M. Stöcker, G. K. Papadopoulos, D. Theodorou, B. Drescher, G. McElhiney, B. Bernauer, V. Krystl, M. Kočiřík, A. Zikánová, H. Jirglová, C. Berger, R. Gläser, J. Weitkamp, E.W. Hansen

149 Zeolite Membranes: Separations Based on Specific Molecular Interactions
J. Kuhn, J. Gross, J.C. Jansen, P.J. Jansens

150 Diffusion in Thermally Fractured Granite Rock Cores Studied by PFG NMR and MRI
Makoto Yamaguchi

151 CO_2 Transport in Amorphous Silica Membranes: Adsorption, Diffusion, and Mitigation of the Effects of Water
R.R. Chance, H.W. Deckman, T.E. Clark, C.J. Yoon, J.A. McHenry, D.C. Calabro, S. Jakubowicz

152 Molecular Transport in Inorganic Membranes: CO_2/CH_4 Separation
E.W. Corcoran, R.R. Chance, H.W. Deckman, G.J. DeMartin, S.C. Reyes, C.J. Yoon, T.E. Clark