

PROGRAMME

Sunday, August 23th

- 16:00 Registration opens at Hotel Emmantina
- 18:00 – 18:15 Welcome (*Doros Theodorou*)
- Oral Session 1: Diffusion in Social Sciences**
- Chair: *Gero Vogl* (Vienna)
- 18:15 – 18:50 The Scaling Laws of Human Travel - From Money Dispersal to Global Disease Dynamics
Dirk Brockmann (Northwestern University, Evanston, Illinois, USA)
- 18:50 – 19:25 Diffusion Models in Anthropology: Population Spread and Cultural Contact
James Steele, Anne Kandler (University College London, United Kingdom)
- 19:25 Welcome Reception, Hotel Emmantina

Monday, August 24th, 2009

Oral Session 2: Diffusion in Polymers

- Chair: *George Fytas* (Heraklion)
- 09:00 – 09:35 Mechanisms and Predictability: Why Fundamentals Matter
Ulrich W. Suter (ETH Zürich, Switzerland)
- 09:35 – 10:10 Diffusion-Controlled Gas Separation Using Polymers
Benny Freeman (University of Texas at Austin, USA)
- 10:10 – 10:45 Beyond Fick: How Best to Deal with non-Fickian Behaviour in a Fickian Spirit
John H. Petropoulos (NCSR "Demokritos", Athens, Greece)
- 10:45 – 11:15 Coffee Break

Oral Session 3: Diffusion in Nanoporous Materials

- Chair: *William S. Price* (Sydney) and *Nick Kanellopoulos* (Athens)
- 11:15 – 11:50 Crossover from Single-File to Fickian Diffusion in Carbon Nanotubes and Nanotube Bundles: Pure Components and Mixtures
Keith E. Gubbins (North Carolina State University, Raleigh, North Carolina, USA)
- 11:50 – 12:25 Diffusion through Porous Media: Ultrafiltration, Membrane Permeation and Molecular Sieving
Douglas Ruthven (University of Maine, Orono, Maine, USA)
- 12:25 – 13:00 The Wealth of Information from Transient Guest Profiles
Jörg Kärger (Universität Leipzig, Germany)
- 13:00 – 14:00 Lunch break
- 14:00 – 16:00 **Poster Session I**
- 16:00 – 23:30 **Excursion** to Cape Sounion and light dinner close to the temple of Sounion

Tuesday, August 25th

Oral Session 4: Diffusion in Nanostructured Solids

Chair: *Helmut Mehrer* (Münster)

- 09:00 – 09:35 Mobile Ions in Nanocrystalline and Amorphous Solids
Paul Heitjans (Leibniz Universität Hannover, Germany)
- 09:35 – 10:10 Diffusion Kinetics in Hollow and Core/Shell Nanoparticles
Graeme E. Murch (University of Newcastle, New South Wales, Australia)
- 10:10 – 10:45 Nanoscale Kirkendall Effect and Beyond
Ulrich Gösele (Max Planck Institute of Microstructure Physics, Halle, Germany)
- 10:45 – 11:15 Coffee Break

Oral Session 5: Dynamics of Systems with Rugged Energy Surfaces

Chair: *Thomas Franosch* (München)

- 11:15 – 11:50 A Simple Mathematical Proof of Boltzmann's Equal *a priori* Probability Hypothesis
Denis J. Evans (Australian National University, Canberra, Australia)
- 11:50 – 12:25 Diffusion Processes in Glass-Forming Systems
Walter Kob (Université de Montpellier II, France)
- 12:25 – 13:00 Mechanical Stability: a Construction Principle for Cells
Klaus Kroy (Universität Leipzig, Germany)
- 13:00 – 14:00 Lunch break
- 14:00 – 16:00 **Poster Session II**
- 20:00 **Conference Dinner**, Roof Garden, Hotel Emmantina

Wednesday, August 26th

Oral Session 6: Diffusion in Living Cells and Tissues

Chair: *Philip Kuchel* (Sydney)

- 09:00 – 09:35 Exploring Diffusional Behaviour in Nanostructured Systems with Single Molecule Probes: From Nanoporous Materials to Living Cells
Christoph Bräuchle (Ludwig-Maximilians-Universität München, Germany)
- 09:35 – 10:10 Diffusion of Helium-3 Gas in Lungs: Understanding Lung Structure and Disease
Mark Conradi (Washington University in St. Louis, Missouri, USA)
- 10:10 – 10:45 Single-Particle Tracking: Connecting the Dots
Michael Saxton (University of California, Davis, USA)
- 10:45 – 11:15 Coffee Break

Oral Session 7: Multiscale Simulations

Chair: *Gunter Schütz* (Jülich)

11:15 – 11:50 Molecular Simulations of Diffusion in Nanoporous Metal-Organic Frameworks
Randall Q. Snurr (Northwestern University, Evanston, Illinois, USA)

11:50 – 12:25 Multiscale Simulation of Perm-Selective Polyelectrolyte Membranes
Alex Neimark (Rutgers University, Piscataway, New Jersey, USA)

12:25 – 14:25 **Poster Session III**

14:25 – 15:30 Light Lunch

15:30 **End of the conference, departures**

POSTER PRESENTATIONS

Poster Session I

Monday, August 24th, 14:00 – 16:00

A – Diffusion in Social Sciences

- A1 Diffusive Interaction in the Clusters of Sinks: Theory and some Applications
Sergey D. Traytak

C – Diffusion in Nanoporous Materials

- C1 Study of the Butane Diffusion in Metal Organic Framework Materials by PFG NMR Experiments
Ziad Adem, Flavien Guenneau, Marie-Anne Springuel-Huet, Antoine Gédéon
- C2 Correlating PFG NMR and IR Diffusion Measurements in Porous Glasses
Ziad Adem, Tobias Titze, Cordula B. Krause, Christian Chmelik, Jens Kullmann, Dirk Enke, Petrik Galvosas, Jörg Kärger
- C3 Dynamics of Electrolyte Solutions Confined in Nanopores
P. -A. Cazade, J. Dweik, B. Coasne, F. Henn, J. Palmeri
- C4 Water in Chabazite Revisited: Self Diffusion and Rotational Relaxation
Rungroj Chanajaree, Philippe A. Bopp, Siegfried Fritzsche, Jörg Kärger
- C5 Bimodal Diffusion of Binary Lennard Jones Mixtures in Atomically Detailed Single-Walled Carbon Nanotubes
Qu Chen, Joshua D. Moore, Ying-Chun Liu, Thomas R. Roussel, Qi Wang, Keith E. Gubbins
- C6 Study of Multi-Component Gas Adsorption by Chromatographic Method and Simulation
Kazuyuki Chihara, Hidenori Nakamura, Yuki Teramura, Yousuke Kaneko
- C7 Diffusion of Chlorinated Hydrocarbons in High Silica Zeolite – Comparison between Chromatographic Data and Molecular Dynamic Simulation
Kazuyuki Chihara, Yuki Teramura, Shinji Tomita, Kenta Saito
- C8 Diffusion of n-Butane/iso-Butane Mixtures in Silicalite-1 Investigated Using Infrared Microscopy
Christian Chmelik, Lars Heinke, Jörg Kärger, Jasper M. van Baten, R. Krishna
- C9 Estimation of Diffusional Rates in Tight Fitting Hydrocarbon-Zeolite Systems
Aldo F. Combariza, German Sastre, Avelino Corma
- C10 Diffusion of Water in LTA Zeolites: a Molecular Dynamics Computer Simulation Study
Pierfranco Demontis, Jorge Gulín-González, Hervé Jobic, Giuseppe B. Suffritti
- C11 Application of the Zero Length Column (ZLC) Technique for Measuring Crystal Diffusivities of the NaX and CeNaX Zeolites
Yasemin Erten, Fehime Çakırcıoğlu-Özkan
- C12 Adsorption-Desorption Kinetics of H₂ molecules on Graphite: a Molecular Dynamics Study
Ole-Erich Haas, Jean-Marc Simon, Signe Kjelstrup
- C13 Assessing Details of Molecular Motion in Nanopores by Combining Different Microscopic Techniques
Lars Heinke, Despina Tzoulaki, Christian Chmelik, Florian Hibbe, Jörg Kärger

- C14 The Coupled Transport of Heat and Mass across a Silicalite Surface.
Non-equilibrium Molecular Dynamics Simulations of n-Butane
Isabella Inzoli, Signe Kjelstrup, Dick Bedeaux, Jean-Marc Simon
- C15 Selective Adsorption of H₂S on MOFs and Zeolite NaX
Bert Jentzsch, Hendrik Kosslick, Henrik Lund, Jörg Harloff, Axel Schulz, Roland Matzmohr, Bertold Sprenger, Hans-Joachim Wolff
- C16 Molecular Dynamics Simulation Study of the Concentration Dependence of the Self-Diffusivity of Methanol in NaX Zeolite
T. Nanok, O. Sangsawang, S. Vasenkov, F. J. Keil, S. Fritzsche
- C17 Molecular Simulation of CO₂ and N₂ Transport in ZSM-5 Zeolite Membranes with Framework Substitutions
David Newsome, Ton Dammers, Marc-Olivier Coppens
- C18 Simulation Studies of CH₄, CO₂, H₂ and D₂ in FAU and MWW Framework Type Zeolites
Evi Pantatosaki, George K. Papadopoulos, Doros N. Theodorou
- C19 PFG NMR Study of Liquid n-Hexane Self-Diffusion in the Bed of Porous Glass Beads
Mikuláš Peksa, Jan Lang, Milan Kočirik
- C20 Diffusion via the Space Discretization (DSD) Method to Study the Concentration Dependence of Self-Diffusion under Confinement
Marco Sant, George K. Papadopoulos, Doros N. Theodorou
- C21 Examining the Reason of the Observed Influence of the Lattice Flexibility on the Diffusion of Ethane in Zn(tbip)
K. Seehamart, T. Nanok, J. Kärger, C. Chmelik, R. Krishna, S. Fritzsche
- C22 Surface Permeabilities: Entering an Unexploited Field by Means of Interference Microscopy
Despina Tzoulaki, Lars Heinke, Florian Hibbe, Jörg Kärger
- C23 Loading Dependent Diffusion Studies on Aromatic Hydrocarbons Adsorbed in MOF-5 via PFG NMR
Markus Wehring, Stefan Hertel, Saeed Amirjalayer, Rochus Schmid, Frank Stallmach
- C24 Assessing the Pore Critical Point of the Confined Fluid by Diffusion Measurement
Philipp Zeigermann, Muslim Dvoyashkin, Rustem Valiullin, Jörg Kärger
- C25 Molecular Traffic Control inside TNU-9 Zeolite
Sakuntala Chatterjee, R. Harish, Gunter M. Schütz
- C26 Diffusion in Ionic Liquids under Geometrical Nano-Confinement
Ciprian Iacob, Joshua R. Sangoro, Rustem Valiullin, Sergej Naumov, Jörg Kärger, Friedrich Kremer
- C27 Dual-Mode Diffusion of Argon Confined in Carbon Nanotube Bundles
Ying-Chun Liu, Thomas J. Roussel, Joshua D. Moore, Qi Wang, Keith E. Gubbins
- C28 In-situ-SANS Investigations of C₅F₁₂ Condensation in Mesoporous Silicas with a Hierarchical Pore Structure
S. Mascotto, B.M. Smarsly, D. Wallacher, A. Brandt
- C29 Slow and Fast (Fickian) Diffusion Modes for Argon Confined in BPL Activated Carbon
Joshua D. Moore, Jeremy C. Palmer, Ying-Chun Liu, Thomas J. Roussel, John K. Brennan, Keith E. Gubbins

- C30 A Combined Atomistic Simulation and Quasielastic Neutron Scattering Study of the Low-Temperature Dynamics of Hydrogen and Deuterium Confined in NaX Zeolite
Evangelia Pantatosaki, George K. Papadopoulos, Hervé Jobic, Doros N. Theodorou
- C31 Analysis of Argon Diffusion in Zeolite Imidazolate Framework-8: Preliminary Calculations
Federico G. Pazzona, Marco Sant, Evangelia Pantatosaki, George K. Papadopoulos, Doros N. Theodorou
- C32 Applying Interference Microscopy to Study Temperature Effects on Molecular Transport in Nanopores
Florian Hibbe, Tomas Binder, Jörg Kärger, Despina Tzoulaki
- C33 Magic-Angle Spinning Pulsed Field Gradient Nuclear Magnetic Resonance (MAS PFG NMR), a New Tool for Diffusometry of Interface Materials
Ekaterina E. Romanova, Moisés Fernández, Farida Grinberg, André Pampel, Jörg Kärger, Dieter Freude

Poster Session II

Tuesday, August 25th, 14:00 – 16:00

B – Diffusion in Polymers

- B1 Helium Permeation through Mixed Matrix Membranes Based on Polyimides and Silicalite-1
Marie Fryčová, Petr Sysel, Pavel Hrabánek, Milan Kočířik, Libor Brabec, Arlette Zikánová, Bohumil Bernauer, Pavel Čapek, Vladimír Hejtmánek
- B2 Tube Geometry and Brownian Dynamics in Semiflexible Polymer Networks
Jens Glaser, Masashi Degawa, Inka Lauter, Rudolf Merkel, Klaus Kroy
- B3 Self-Diffusivity and Free Volume: an Ideal Binary Mixture
Ryan J. Larsen, Charles F. Zukoski
- B4 Experimental Investigation of the Release Mechanism of Hydrophilic Solutes from Hydrophobic Matrices
Dimitrios N. Soulas, Kyriaki G. Papadokostaki
- B5 Mechanisms of non-Fickian Micromolecular Diffusion in Glassy Polymer Films: Analysis of Experimental Sorption and Concurrent Dilation Kinetics in the Light of a Differential Swelling Stress Model
Dimitrios F. Stamatialis, Dimitrios N. Soulas, Merope Sanopoulou
- B6 Microscopic Diffusion Mechanism of CO₂ in a Glassy Amorphous Polymer Matrix
Niki Vergadou, Doros N. Theodorou
- B7 Novel High Free Volume Polymer, Addition Polytrimethylsilylnorbornene: Diffusion or Solubility Controlled Permeation
Yu. Yampolskii, L. Starannikova, N. Belov, M. Galizia, M.G. De Angelis, G.C. Sarti
- B8 Broadband Dielectric Spectroscopy as a Tool to Study Diffusion Coefficients in Conducting Glass-Forming Systems
Joshuha R. Sangoro, Ciprian Iacob, Sergej Naumov, Jörg Kärger, Friedrich Kremer
- B9 Dispersive Gaussian Hole Transport in a Molecularly Doped Polymer
N. Schupper, R. Kahatabi, R. Diamant, D. Avramov

D – Diffusion in Nanostructured Solids

- D1 Absolute Diffusion Rates in Minerals of the Earth Lower Mantle from First Principles
Michael W. Ammann, John P. Brodholt, Andrew J. Walker, David P. Dobson
- D2 Limits of the Ratios of Tracer Diffusivities for the Vacancy-Pair Mechanism with Application to Compound Semi-Conductors
I.V. Belova, D. Shaw, G.E. Murch
- D3 Ultra-Fast Diffusion in Severely Deformed Materials
S.V. Divinski, J. Ribbe, G. Replitz, Y. Estrin, G. Wilde
- D4 Ionic Transport in Mechanosynthesized Nanocrystalline LiBaF₃
Andre Düvel, Martin Wilkening, Paul Heitjans
- D5 Li Diffusion in Li₂Ti₃O₇ Probed by ⁷Li Stimulated Echo NMR
Jessica Heine, Martin Wilkening, Paul Heitjans
- D6 Modeling of Diffusion Saturation of Titanium by Nitrogen Taking into Consideration Structural and Phase Transformations
Ya. Matychak, V. Fedirko, I. Pohrelyuk, O. Tkachuk

- D7 Diffusion under a Stress in Interstitial Alloys and Simulation of Atom Redistribution near the Crack Tip
Andrei V. Nazarov, A.A. Mikheev, M.U. Ryabov, A.G. Zaluzhnyi
- D8 On the Physics of Some Known Diffusion Anomalies in Metallic and Carbonaceous Systems
Yury S. Nechaev
- D9 Dynamic of Defects in an Iron Monolayer on W (110)
E. Partyka-Jankowska, B. Sepiol, F. Gröstlinger, G. Vogl, J. Korecki, T. Ślęzak, M. Zajac, A. Chumakov
- D10 Molecular Dynamics Simulation of Atomic Structure in the Vicinity of Point Defects in FCC and BCC Metals
Alena Rashetnikava, Alexander Germanov, Irina Valikova, Andrei Nazarov
- D11 Simulation of Pressure- and Temperature Dependence of Impurity Diffusion in BCC Metals
Irina Valikova, Andrei Nazarov
- D12 Use of Time Resolved X-ray Radiography to Measure Interdiffusion in Liquid Metals
B. Zhang, A. Griesche, A. Meyer
- D13 A Molecular Dynamics Study of Anisotropic Oxygen Diffusion in $\text{La}_2\text{NiO}_{4+\delta}$
Alexander Chroneos, David Parfitt, John A. Kilner, Robin W. Grimes
- D14 Contribution to the Understanding of the Point Defect Influence on some Transport Properties in UO_{2+x}
Fatma Riahi, Sofiane Laouar, Djamel Eddine Mekki
- D15 Influence of Defect Clusters on Diffusion Processes in UO_{2+x}
Fatma Riahi, Djamel Eddine Mekki
- D16 Migration Mechanism in Defect Metal Hydrides Containing Superabundant Vacancies
Hidehiko Sugimoto, Yuh Fukai

E – Dynamics of Systems with Rugged Energy Surfaces

- E1 Diffusion-Localization and Liquid-Glass Transitions of a Colloidal Fluid in Porous Confinement
Daniele Coslovich, Dieter Schwanzer, Gerhard Kahl
- E2 Cluster-Resolved Dynamic Scaling Theory and Universal Corrections for Transport on Percolating Systems
Thomas Franosch, Felix Höfling
- E3 Propagation of Solid-Liquid Interfaces in Disordered Linear Pores
Daria Kondrashova, Alexey Khokhlov, Rustem Valiullin, Jörg Kärger
- E4 Memory Effects in Confined Fluids via Diffusion Measurement
Sergej Naumov, Rustem Valiullin, Jörg Kärger, Peter A. Monson
- E5 Diffusion and Segmental Dynamics of Double-Stranded DNA
Eugene P. Petrov, Roland G. Winkler, Petra Schwille
- E6 Atomic Motion in Metallic Glass Studied by Coherent X-Rays
Bogdan Sepiol, Michael Leitner, Bastian Pfau, Friedrich Gröstlinger, Lorenz-Mathias Stadler
- E7 Surface Diffusion of Particles over the Bivariate Trap Lattices
Alexander Tarasenko, Lubomir Jastrabik

- E8 Energy Landscape–Based Study of Atomic Displacements in Glass Forming Materials
Dimitrios Tsalikis, Nikolaos Lempesis, Georgios C. Boulougouris, Doros N. Theodorou
- E9 Localization and Glass Formation of Fluids Confined in Porous Matrices
Jan Kurzidim, Daniele Coslovich, Gerhard Kahl

Poster Presentation III

Wednesday, August 26th, 12:25 – 14:25

F – Diffusion in Living Cells and Tissues

- F1 Measuring Molecular Exchange for Water in a Yeast Cell Suspension through NMR Diffusometry
Ingrid Åslund, Samo Lasič, Agnieszka Nowacka, Markus Nilsson, Daniel Topgaard
- F2 Investigations of Static and Dynamic Heterogeneities in Ultra-Thin Liquid Films via Scaled Squared Displacements of Single Molecule Diffusion
Michael Bauer, Mario Heidernätsch, Daniela Täuber, Jörg Schuster, Christian von Borczyskowski, Günter Radons
- F3 Simulating Hot Nano Beads
Dipanjan Chakraborty, Frank Cichos, Klaus Kroy
- F4 A First Passage Time Approach to Diffusion in Liquids
A.J. Dammers, V.J. van Hijkoop, M.-O. Coppens
- F5 A Fractal Based Model of Diffusion MRI in Cortical Grey Matter
Brian Hansen, Leif Østergaard, Peter Vestergaard-Poulsen
- F6 Diffusive Dynamics in Protein Solutions Studied by Neutron Spin Echo
W. Häußler, B. Gohla-Neudecker
- F7 Hot Brownian Motion
Daniel Rings, Romy Radünz, Frank Cichos, Klaus Kroy
- F8 Discrimination between Static and Dynamic Heterogeneities in Single Dye Diffusion in Ultrathin Liquid Films
Daniela Täuber, Jörg Schuster, Mario Heidernätsch, Michael Bauer, Günter Radons, Christian von Borczyskowski
- F9 NMR Diffusive Diffraction Studies of Emulsions
Nirbhay N. Yadav, William S. Price
- F10 Translational Diffusion in Two-Component Lipid Membranes Close to Phase Transition: A Monte Carlo Study
Jens Ehrig, Eugene Petrov, Petra Schwille
- F11 Shear-flow mediated changes in DNA morphology
Katrin Günther, Kristin Laube, Michael Mertig
- F12 An Advanced Method of Tracking Temporarily Invisible Particles in Video Imaging
Mario Heidernätsch, Michael Bauer, Daniela Täuber, Günter Radons, Christian von Borczyskowski
- F13 DNA Interaction with Freestanding Cationic Lipid Bilayers
Christoph Herold, Eugene P. Petrov, Petra Schwille
- F14 Fast MRI for Spatially Resolved Quantitative Information on Molecular Exchange
Samo Lasič, Ingrid Åslund and Daniel Topgaard

- F15 Diffusion Measured with Scanning Fluorescence Correlation Spectroscopy
Zdeněk Petrášek, Susan Derenko, Petra Schwille
- F16 Investigation of Solid Liquid Interface in Ultra-Thin Liquid Films via Single Particle Tracking of Colloidal Particles
Ines Trenkmann, Jörg Schuster, Shubhra Gangopadhyay, Christian von Borzyskowski

G – Multiscale Simulations

- G1 3D Stochastic Replicas of Porous Solids: A Way to Improve Predicted Diffusivity
P. Čapek, V. Hejtmánek, L. Brabec, A. Zikánová, M. Kočířik, B. Bernauer
- G2 Diffusion in Uniform and Modulated Porous Silicon Channels
Muslim Dvoyashkin, Alexey Khokhlov, Rustem Valiullin, Jörg Kärger
- G3 Simulation of N₂/CH₄ Counter-Diffusion in Composite Membranes of the Type Silicalite-1- α-Alumina
Vlastimil Fila, Milan Kočířik, Pavel Hrabánek, Arlette Zikánová, Libor Brabec, Bohumil Bernauer
- G4 Measurement and Modeling of Mass Transport in Porous Composite Structures for Adsorption Heat Pumps
Gerrit Földner
- G5 Kinetics of Pyridine Adsorption onto Granular Activated Carbon
Roberto Leyva-Ramos, Raul Ocampo-Perez, Oliva L. Torres-Rivera, Maria S. Berber-Mendoza, Nahum A. Medellin-Castillo
- G6 Kinetics of Fluoride Adsorption onto Bone Char
R. Leyva-Ramos, N.A. Medellín-Castillo, J. Mendoza-Barron, Laura Fuentes-Rubio, Rosa M. Guerrero-Coronado, Raul Ocampo-Perez
- G7 Diffusion in Hierarchical Pore Systems
Sergej Naumov, Rustem Valiullin, Jörg Kärger, Bernd Smarsly
- G8 3D X-ray CT and Diffusion Measurements to Assess Tortuosity and Constrictivity in a Sedimentary Rock
Hiroaki Takahashi, Yoshimi Seida, Mikazu Yui