ESF-Science Meeting

DIFFUSION FUNDAMENTALS III

organized in Athens, Greece
23-26 August, 2009

by

Christian Chmelik, University of Leipzig, Germany
Jörg Kärger, University of Leipzig, Germany
Nick Kanellopoulos, NCSR "Demokritos", Athens, Greece
Doros N. Theodorou, National Technical University of Athens, Greece

FINAL REPORT

Summary

"Diffusion Fundamentals III" was the third in a series of biannual international conferences designed to bring together researchers from the physical, chemical, biological, materials, and social sciences in order to discuss advances in theory, computer simulations, experimental measurements, and technological applications of diffusion phenomena and fertilize the development of ideas and collaborations across different disciplines.

"Diffusion Fundamentals III" took place in Glyfada, near Athens, Greece from the 23rd to the 26th of August, 2009. It attracted 119 participants and 11 accompanying members. Although this was a predominantly European conference, 22% of the participants came from North and Central America, Oceania, Asia, and Africa. Participants formed a multidisciplinary group composed of physicists, chemists, materials scientists, chemical engineers, molecular biologists, and even archaeologists. Roughly one third of the participants were doctoral students.

The themes selected for "Diffusion Fundamentals III" were Diffusion in the Social Sciences; Diffusion in Polymers; Diffusion in Nanoporous Materials; Diffusion in Nanostructured Solids; Dynamics in Systems with Rugged Energy Surfaces; Diffusion in Living Cells and Tissues; and Multiscale Simulations of Diffusion Processes. The format followed previous "Diffusion Fundamentals" conferences: The entire conference was plenary (no parallel sessions). There were 19 invited lectures of duration 35 minutes by world-recognized experts in the various themes and 92 poster presentations. A session was dedicated to each theme. Following the tradition of Diffusion Fundamentals conferences, session chairmen and invited speakers highlighted posters relevant to their sessions and lectures, respectively. Another tradition of Diffusion Fundamentals conferences which was kept in this conference is the Conference Book, containing original articles by the invited speakers and session chairmen, as well as extended abstracts of all posters accepted for presentation at the time of publication, and adorned with watercolors of the venue (Athens) by participant Taro Ito of Sapporo, Japan.

The general consensus among participants, upon conclusion of the conference, is that it was highly successful. The conference room was packed until the very end. Most invited speakers and poster presenters did an excellent job introducing their subject to the multidisciplinary audience, pointing out links to other areas of diffusion research and conveying the excitement and promise of their work. There were a lot of excellent questions and lively discussion after the talks, in front of the posters, and during meals. Ideas for collaboration were put forth by participants with complementary expertise. Thus, despite the broad spectrum of themes covered and the diverse backgrounds of the participants, the conference was remarkably coherent. In the words of a participant, the conference reinforced the feeling of belonging to a "family" of diffusion researchers. It also encouraged the exchange of new experimental, theoretical, and simulation tools to improve our understanding of diffusion-related phenomena that are key to public health, energy production, new materials, and protection of the environment.

Description of the Scientific Content of and the Discussion at the Event

Diffusion phenomena play a key role in materials science and biology, but also in physics, physical chemistry, chemical engineering, medical diagnostics, epidemiology, and anthropology. A search of *Current Contents* reveals more than 10,000 publications per year on various aspects of diffusion. Scientists in different fields often face similar challenges in the theoretical analysis, computer simulation, experimental measurement, and engineering design of systems dominated by diffusion phenomena. Nevertheless, they are often unaware of each other's work. There is tremendous benefit to be gained from bringing these scientists together and stimulating a cross-fertilization of ideas across different disciplines.

With this in mind, the series of international conferences on *Diffusion Fundamentals* was started in 2005. The inaugural year of the conferences coincided with the 150th anniversary of Adolf Fick's *Über Diffusion* (1855) and with the 100th anniversary of Albert Einstein's *Über die von der molekularkinetischen Theorie der Wärme geforderten Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen* (1905). The first conference in the series took place in Leipzig, the city where both of these seminal papers on diffusion were originally published. The Leipzig conference, organized by Jörg Kärger, Farida Grinberg, and Paul Heitjans, took place September 22-24, 2005 and was highly successful. Proceedings from the Leipzig conference were published in *Diffusion Fundamentals*, Leipziger Universitätsverlag, Leipzig, 2005, ISBN 3-86583-073-0. The second conference in the series, *Diffusion Fundamentals II*, was organized by Stefano Brandani, Christian Chmelik, Jörg Kärger, and Roberto Volpe in L' Aquila, Italy in August 26-29, 2007. Again, it was highly successful. Its proceedings were published in *Diffusion Fundamentals II*, Leipziger Universitätsverlag, Leipzig, 2007, ISBN 978-3-86583-209-2.

Following the recommendation of the International Scientific Committee, *Diffusion Fundamentals III* was organized in Athens, Greece August 23-26, 2009. The conference chairmen were Christian Chmelik of the University of Leipzig, Germany; Jörg Kärger of the University of Leipzig, Germany; Nick Kanellopoulos of NCSR "Demokritos", Athens, Greece; and Doros N. Theodorou of the National Technical University of Athens, Greece. They were assisted by organizing teams consisting of members of their research groups, most notably Tomas Binder of the University of Leipzig; George Romanos and Niki Vergadou of NCSR "Demokritos"; and George Papadopoulos of NTU Athens. Athens was chosen in the spirit of looking for venues that combine a rich scientific and cultural heritage, such as Leipzig and L' Aquila; also, venues where a "low budget" conference emphasizing scientific fundamentals would be affordable.

Seven themes were set for Diffusion Fundamentals III by the organizers, after consultation with the International Scientific Committee. These were:

A. Diffusion in the social sciences
B. Diffusion in polymers
C. Diffusion in nanoporous materials
D. Diffusion in nanostructured solids
E. Dynamics in systems with rugged energy surfaces
F. Diffusion in living cells and tissues
G. Multiscale simulations of diffusion phenomena

The purpose of the conference was to highlight recent advances, challenges, and opportunities in theoretical, simulation, and experimental work aimed at enhancing our fundamental understanding of diffusion phenomena in the broad range of material, biological, cellular, environmental, social, and financial systems relevant to the seven themes listed above; also, at using this understanding in applications. Problems and methods were to be discussed both by theme and horizontally, across different disciplines, in a manner that would promote cross-fertilization among the disciplines.

The format of the Athens conference followed previous Diffusion Fundamentals conferences. There were no parallel sessions. The entire programme was plenary, consisting of invited lectures and poster presentations. 19 speakers (3 per theme for themes B to F and 2 per theme for themes A and G) were carefully chosen and invited in October 2008 to give lectures in a 30 min. talk plus 5 min. discussion format. Submission of poster presentations was opened through the conference web page http://www.diffusion-fundamentals.org in January 2009. Seven sessions corresponding to the seven themes were set up, and distinguished scientists were invited to chair these sessions. Following the tradition of Diffusion Fundamentals conferences, session chairmen and invited speakers were asked to highlight posters relevant to their sessions and lectures, respectively. Again following tradition, session chairmen and invited speakers were asked to contribute full papers to the Conference Book, in which extended abstracts of poster presentations also appeared.

Diffusion Fundamentals III was conducted in Glyfada, Athens, Greece according to the programme appearing at the end of this report. Below we provide a brief description of the scientific content and the discussions in each of the seven sessions:

A. *Diffusion in the Social Sciences*.
The inaugural invited talk discussed how scaling laws for human travel can be formulated, with particular reference to the “where’s George” experiment of tracking the trajectories of individual dollar bills across the USA. In today’s world of long-range air travel, the trajectories of dollar bills exhibit characteristics reminiscent of Lévy flights, the probability density for observing a displacement r within a week scaling as $r^{-1.6}$. Assuming that the flux of currency is representative of the flux of humans, models for human mobility formulated in this way can be combined with simple models of infection (e.g., the SIR, or Susceptible-Infected-Recovered model) in order to predict the spread of epidemics. Simulations of the spread of swine flu across the continental USA were presented, based on these ideas. Another subject

highlighted in this session was the use of diffusion models to deal with population spread and cultural contact in Anthropology. Partial differential equation models were presented for the spread of early farming in pre-historic societies, for the diffusion of innovations, and a more elaborate model was discussed for the fate of endangered languages, using the Gaelic-English competition in Scotland as a case study.

B. *Diffusion in Polymers*

How local inhomogeneities give rise to anomalous diffusion in polymers over times that may exceed the microsecond range was discussed. Simulation strategies based on analysis of infrequent events (transition-state theory) were reviewed for the prediction of diffusivity of small-molecule penetrants in polymers in cases where diffusion is too slow to be tracked reliably by molecular dynamics (MD). Applications of polymer membranes for the diffusion-controlled separation of industrial gas mixtures, such as CO_2/H_2 , were discussed. Practical examples of designing membrane polymers so as to control the molecular flexibility, polarity, crystallinity, and free volume distribution and thereby achieve combinations of permeability and selectivity that exceed the "Robeson limit" characterizing conventional polymeric materials were presented. For cases with strongly concentration dependent diffusivities (e.g., CCl_4 or CF_2Cl_2 in silica), simple formulations "in a Fickian spirit" employing the gradient of chemical potential as a driving force were presented. For cases where diffusion takes place in a relaxing medium (e.g. solvent diffusing into a glassy polymer, causing swelling of the polymer) observed behaviour can be explained with simple models which take into account the kinetics of relaxation along with diffusion; examples where normal and "Case II" diffusion may coexist in the same oriented polymer sample were discussed.

C. *Diffusion in Nanoporous Materials*

The first talk in this session showed how molecular dynamics simulations can be used to explore single-file diffusion effects of noble gases and water within single-walled carbon nanotubes. The mechanism and rate of motion of each of these small molecules in the nanotube were quantified for various nanotube diameters and chiralities (zigzag, armchair). Diffusion in bundles of nanotubes was also explored. The second talk reviewed the conditions under which selectivity can be achieved in reverse osmosis and ultrafiltration separations using inorganic membranes. The validity of the Knudsen diffusion model of selectivity was discussed for separations employing mesoporous silica membranes. The function of molecular sieving membranes was illustrated through the examples of CO_2/CH_4 and C_2H_6/CH_4 separations. The third talk clarified the distinction between transport diffusion, self-diffusion by tracer exchange, and self-diffusion measurements. It then discussed interference microscopy and FTIR micro-imaging studies of transient diffusion profiles within individual zeolite crystals and the wealth of information that is obtained from these studies concerning transport diffusivities, surface permeabilities, and their dependence on defects and barriers to transport on the surface of and within the crystals.

D. *Diffusion in Nanostructured Solids*
Recent advances in Monte Carlo and molecular dynamics simulations for understanding the Kirkendall effect, involving the spontaneous formation of voids in binary solids where the components differ very much in diffusivity, were discussed. Simulations were presented to explore how the Kirkendall effect can be utilized for the formation of hollow nanospheres (e.g., of Pt) or core-shell nanoparticles (e.g., Ag-Ni, Ni-Pd) and for the spark ignition of laminated nanofoils (e.g. Ni-Ag). Other diffusion-related phenomena relevant to nanotechnological applications that were discussed, mainly at an experimental level, included atomic layer deposition, Rayleigh instability combined with atomic layer deposition, the formation of hollow SiO_2 nanospheres by oxidation of Si nanoparticles in water, and the diffusion of metals into spider silk. The unique mechanical and electronic properties of the materials obtained through these processes were discussed.

E*. Dynamics of Systems with Rugged Energy Surfaces*
This session reviewed some important theoretical developments in statistical mechanics: The fluctuation theorem governing fluctuations in the sign of entropy production (apparently violating the second law of thermodynamics) in systems with finite number of particles; the resolution of Loschmidt's objection to Boltzmann's entropy production argument, based on the idea that for every trajectory in phase space there is a corresponding anti-trajectory; the dissipation theorem and the relaxation theorem governing the temporal evolution of the distribution of dynamical systems in phase space. Diffusion processes in glass-forming systems were discussed next. The peculiar temperature dependence of transport coefficients and the physical origin of the ballistic, β-relaxation, and α-relaxation regions in the time dependence of the intermediate structure factor were clearly reviewed. Next, a simple computer model of hard cubes on a three-dimensional cubic lattice was considered and it was shown that glassy dynamics results from the imposition of simple rules for the motion of these cubes, depending on the number of their neighbours. "Active sites" in the model system were defined in terms of the traffic of particles passing through them and the cluster distribution of these sites was analyzed, exhibiting percolation at long times. The van Hove correlation function of moving particles was shown to conform to a continuous time random walk model with a Gaussian distribution of local vibrational displacements, a Gaussian distribution of longer (diffusional) jump lengths, and an exponential distribution of waiting times between jumps. At intermediate times, the van Hove correlation function exhibits an exponential dependence on displacement. In the same session, models based on wormlike chains were put forth to explain the mechanics of actin networks present in the cytoskeleton (mechanical response to pulling tissue) and the rheological properties of actin solutions.

F. *Dynamics of Living Cells and Tissues*
Principles and applications of single molecule spectroscopy were introduced. Results were presented from investigating the mechanism of single molecule dynamics (translation, rotation, trapping, spectral diffusion) in nanoporous materials; controlled release of drugs from novel drug delivery systems based on mesoporous silica; and tracing of single viruses as they enter a cell and

are transported to the nucleus. Imaging the restricted diffusion of ^{3}He in the gas spaces of the lungs was discussed as a remarkably sensitive and discriminating diagnostic technique for understanding emphysema. The diameters of the tubes constituted by adjacent alveolar sacs can be measured through a simple model of anisotropic diffusion. The connectivity of airways in the lung can be explored through measurements of long-range diffusion of ^{3}He; these measurements bring out the importance of collateral paths in the lung.

G. *Multiscale Simulations of Diffusion Phenomena*
Atomistic simulations of sorption and diffusion of C_1 to C_{16} alkanes, aromatic hydrocarbons, and CO_2 in Metal Organic Framework (MOF) materials were presented. Calculations with relatively simple force fields are in very good agreement with available experimental data and elucidate the siting and modes of motion of sorbates in this versatile category of materials, which shows great promise for industrial separations. In many cases simulation has preceded experimental measurement of sorption and transport in these novel materials. An interesting finding from simulations, which is confirmed by experimental measurements, is that isoreticular MOFs exhibit a negative thermal expansion coefficient. Another interesting category of materials in which diffusion is of paramount importance is permselective polyelectrolyte membranes (Nafion, sulfonated polystyrene – poly(1-butene) – polystyrene triblock copolymers). These are being considered as materials for protective clothing of soldiers. They are water permeable, but at the same time can block phosphorus-containing organic compounds, which are very soluble in water. A multiscale modelling strategy is necessary for understanding the unique permeation properties of these materials, because of their complex microphase-separated morphology. One such strategy was outlined, utilizing atomistic MD, coarse-grained Monte Carlo, mesoscale dissipative particle dynamics (DPD) for predicting the morphology, and kinetic lattice Monte Carlo for estimating transport properties.

Assessment of the Results and Impact of the Event on the Future Direction of the Field

Diffusion Fundamentals III was attended by 119 participants and 11 accompanying members. Attendance was close to the target originally set in planning the conference, despite unforeseen adverse developments (financial crisis, swine flu) in 2008-2009. The distribution of the 119 participants by nationality is shown in Table 1. The highest participation came from Germany, Greece, and the United States. Although this was predominantly a European conference, 22% of the participants came from North and Central America, Oceania, Asia, and Africa. Participants constituted a multidisciplinary group composed of physicists, chemists, materials scientists, chemical engineers, molecular biologists, and even archaeologists. Roughly one third of the participants were doctoral students.

Table 1: Distribution of participants by country

Country	*Participants*	*Country*	*Participants*
Algeria	1	Italy	2
Australia	6	Japan	4
Austria	5	Mexico	2
China	1	Netherlands	1
Czech Republic	3	Russia	1
Denmark	1	Slovenia	1
France	4	Spain	1
Germany	54	Sweden	2
Greece	14	Switzerland	1
India	1	United Kingdom	3
Israel	1	U.S.A.	10

The conference was highly successful. This is attested by the fact that the lecture room, where the 19 invited lectures were given, was full until the very end and by the lively discussion that took place after the lectures and in front of the 92 posters presented. Following the recommendations of the organizers, lecturers and poster presenters tried seriously (and successfully) to place their work in a broader context, make it understandable to a general audience, and establish connections with other diffusion sub-fields. Also, most conference chairmen and invited speakers did an excellent job summarizing the posters relevant to their session or lecture and highlighting new ideas that emerged from them. As a consequence, all participants were able to follow the presentations comfortably and contribute valuable comments, despite the diversity of their backgrounds.

Some conclusions that can be made on the basis of presentations and discussions at Diffusion Fundamentals III are the following:

- The mobility of humans, the spreading of diseases, the competition between languages, and a wide variety of other phenomena in epidemiology and the social sciences are amenable to quantitative modelling and simulation with methods similar to the ones developed in the physical sciences. Scaling laws comparable to the ones observed in physical phenomena are often observed in these areas, and need to be understood on a more fundamental level. The reliable collection of data is important for parameterizing and refining the models, and thereby enhancing their reliability.
- Membrane processes employing polymers are gaining ground in conducting industrial separations, flue gas and waste treatment in environmentally friendly and energy-efficient way. Molecular design of the chemical constitution of the polymers is important for achieving the permeability and selectivity needed in these applications. Monte Carlo, molecular dynamics, and transition state theory-based methods can help in this molecular design. Simple nonequilibrium thermodynamics-based models incorporating the stress state of and structural relaxation in the

polymer can be used to understand complex non-Fickian diffusion phenomena in polymer/solvent systems.

- Thanks to advances in interference microscopy and FTIR micro-imaging of transient diffusion profiles within individual crystals, along with pulsed-field gradient NMR measurements, it is now possible to measure transport, self-, and long-range diffusivities as well as surface permeabilities of fluid molecules in nanoporous solids, such as zeolites, with unprecedented accuracy, and to quantify how these transport phenomena depend on defects and barriers to transport on the surface of and within the crystals and on the packing and binding between crystals.
- The Kirkendall effect and a host of other diffusion-related phenomena can serve as a basis for the development of nanostructured solids with unique constitution, morphology and properties.
- A continuous time random walk model with a Gaussian distribution of local vibrational displacements, a Gaussian distribution of longer (diffusional) jump lengths, and an exponential distribution of waiting times between jumps can capture the mean squared displacement across the β and α relaxation regimes in computer simulations of simple models of glass-forming materials. According to these simulations, the α relaxation is associated with a percolation of "active" domains, where molecular motion is most pronounced.
- Single molecule spectroscopy is a powerful tool for understanding the mechanism of transport phenomena and for probing structure over a variety of length scales in materials and biological systems.
- Imaging the restricted diffusion of ^{3}He in the gas spaces of the lungs is a remarkably sensitive and discriminating surgery-free diagnostic technique for understanding and treating emphysema. Valuable structural information about the lungs can be extracted by constructing simple models of the diffusion process. This novel technique illustrates the great importance of diffusion measurements in medical diagnostics.
- Molecular simulation strategies for the prediction of sorption and diffusion of gases in zeolites can be carried over to novel nanoporous materials, such as Metal Organic Frameworks, providing a wealth of mechanistic information on the molecular processes that govern sorption capacity and selectivity. As these materials are quite new, simulation studies of sorption and transport in them often precede experimental measurements; thus, simulation has a chance to contribute to the rational design of these materials.

An important output of Diffusion Fundamentals III was the Conference Book, "Diffusion Fundamentals III", edited by Christian Chmelik, Nick Kanellopoulos, Jörg Kärger, and Doros Theodorou, Leipziger Universitätsverlag, ISBN 978-3-86583-387-7. The book contains chapters contributed by the invited speakers and conference chairmen, including an introductory chapters on "Heroes and Highlights in the History of Diffusion" by Helmut Mehrer and Nicolaas Stolwijk. It also contains extended abstracts of all posters accepted for presentation at the time the book was sent to the publisher. A more complete version, including all poster abstracts, will appear on the web site of the online journal Diffusion Fundamentals. As has become a tradition in Diffusion Fundamentals conference, the Conference Book contains reproductions of 25

exquisite water colours of the venue (Athens) painted specifically for the conference by participant physicist/artist Taro Ito of Sapporo, Japan. These paintings are used as a starting point for a brief discussion of the history of Athens and of the session themes. This unique structure imparts to the conference book considerable artistic and cultural, as well as scientific value. The contents of the conference book are available at http://www.uni-leipzig.de/diffusion/df3-conference-volume/DFIII_complete.pdf and the book cover can also be downloaded from the URL http://www.uni-leipzig.de/diffusion/df3-conference-volume/DFIII_cover.pdf.

In Athens the International Scientific Committee decided that the next Diffusion Fundamentals conference, the fourth in the series, will take place in the vicinity of Troy, in upstate New York State, USA in August 2011. Diffusion Fundamentals IV will be organized by Prof. Marc-Olivier Coppens of Rensselaer Polytechnic Institute in Troy, NY; Professor Douglas Ruthven of the University of Maine in Orono, ME; Professor Alexander Neimark of Rutgers University, NJ; and Dr. Matthias Thommes of Quantachrome Instruments, Inc. The fact that the conference migrates away from the European continent for the first time in its history is indicative of the state of maturity it has reached and of its growing international status and impact.

Final Programme of the Meeting

Diffusion Fundamentals III

Basic Principles of Theory, Experiment and Application

August 23th to 26th, 2009
Athens, Greece

SCHEDULE

Sunday, August 23th

16:00	Registration opens at Hotel Emmantina
18:00 – 18:15	Welcome (Doros Theodorou)
18:15 – 19 :25	Oral Presentations
19:25	Welcome Reception, Hotel Emmantina

Monday, August 24th

09:00 – 16:00	Oral and Poster Presentations
16:00 – 23:30	Conference Excursion

Tuesday, August 25th

09:00 – 16:00	Oral and Poster Presentations
20:00	Conference Dinner, Roof Garden, Hotel Emmantina

Wednesday, August 26th

09:00 – 14:25	Oral and Poster Presentations
15:30	End of the Conference

All oral sessions are held in the Hotel Emmantina Conference Room. All poster sessions take place in the Hotel Emmantina salons.
Please find the detailed programme on page 14.

ORGANIZATION

Conference Chairmen: Christian Chmelik, Leipzig; Nick Kanellopoulos, Athens;
Jörg Kärger, Leipzig; Doros Theodorou, Athens

Organizing Committee / Editorial Board: Dezsö L. Beke, Debrecen
Stefano Brandani, London/Edinburgh
Armin Bunde, Gießen
Paul Callaghan, New Zealand
Alan Chadwick, Canterbury
Marc-Olivier Coppens, Delft
Gerhard Ertl, Berlin
Dieter Freude, Leipzig
Farida Grinberg, Leipzig
Paul Heitjans, Hanover
Jörg Kärger, Leipzig
Yossi Klafter, Tel Aviv
Alfred Leipertz, Erlangen-Nürnberg
Graeme Murch, Callaghan
Jean Philibert, Paris
William S. Price, Sydney
Douglas M. Ruthven, Orono
Michael J. Saxton, Davis
Gunter Schütz, Jülich
Doros Theodorou, Athens
Ilpo Vattulainen, Helsinki
Gero Vogl, Vienna
George H. Weiss, Bethesda

Organizing Team Athens: George Romanos, George Papadopoulos, Niki Vergadou

Phone +30 210 6503 981, Fax +30 210 6535 294,
Mobile +306936900092
E-mail: groman@chem.demokritos.gr

Organizing Team Leipzig: Christian Chmelik, Tomas Binder
Phone +49 341 97 32531, Fax +49 341 97 32549
E-mail: info@diffusion-fundamentals.org

Conference Office / Registration Desk:

Sunday, August 23th	15:00 – 22:00
Monday, August 24th	8:30 – 14:00
Tuesday, August 25th	8:30 – 16:00
Wednesday, August 26th	8:30 – 13:00

Conference Venue: Emmantina Hotel
Glyfada, 166 75 Athens, Greece

SCOPE

Diffusion involves the irregular movement of particles and is among the fundamental, omnipresent phenomena of nature. It occurs in all states of matter and is critically important to many technological processes as well as for the functioning of living cells. Even the propagation of diseases, men and ideas may be considered as diffusion phenomena.

Two years after Diffusion Fundamentals II in L'Aquila, Italy, and as part of the celebration of the 600th anniversary of the foundation of Leipzig University, the cradle of the Diffusion Fundamentals Conference series in 2005, the world-wide community of researchers in the field of diffusion is invited to Athens, Greece, to highlight current developments. Following the tradition of Diffusion Fundamentals I and II a Conference Volume with paintings of Athens by the Japanese physicist and artist Taro Ito will appear as a souvenir for all participants. Diffusion Fundamentals III is organized under the auspices of the National Technical University of Athens, the National Centre for Scientific Research “Demokritos”, and the University of Leipzig.

The scientific programme consists of 19 plenary lectures. They are scheduled to provide an introduction into the many diverse fields of relevance for diffusion theory, experiment and application, and will be accompanied by examples of the hot topics of current research. About 90 posters will illustrate the large spectrum of research activities. Poster presenters are kindly asked to hang their posters early in the morning of the day to which they have been assigned (see pages 7-12) and to take them down by 18:00 of the same day. Each poster should be displayed on the board bearing its number. Presenters are also kindly asked to make themselves available by their posters for discussion during the designated sessions.

Each group of plenary talks will be accompanied by poster sessions. Ideally, the contributions to the poster sessions should be related to the various aspects covered in the plenary talks. Correspondingly, the plenary speakers and the chairpersons of the sessions were asked to serve as first reviewers of the poster submissions and were encouraged to refer to individual posters during their presentations, whenever appropriate.

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 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 Çakıcıoğlu-Özkan

C12 Adsorption-Desorption Kinetics of H_2 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 H_2S 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 CO_2 and N_2 Transport in ZSM-5 Zeolite Membranes with Framework Substitutions
David Newsome, Ton Dammers, Marc-Olivier Coppens

C18 Simulation Studies of CH_4, CO_2, H_2 and D_2 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 Kočiřík

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 C_5F_{12} 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 Kočiřík, 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 CO_2 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. Reglitz, Y. Estrin, G. Wilde

D4 Ionic Transport in Mechanosynthesized Nanocrystalline $LiBaF_3$
Andre Düvel, Martin Wilkening, Paul Heitjans

D5 Li Diffusion in $Li_2Ti_3O_7$ Probed by ^{7}Li 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. Sepiol1, F. Gröstlinger, G. Vogl, J. Korecki, T. Ślęzak, M. Zając, 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 $La_2NiO_{4+\delta}$
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 Borcyskowski

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 Borczyskowski

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. Kočiřík, B. Bernauer

G2 Diffusion in Uniform and Modulated Porous Silicon Channels
Muslim Dvoyashkin, Alexey Khokhlov, Rustem Valiullin, Jörg Kärger

G3 Simulation of N_2/CH_4 Counter-Diffusion in Composite Membranes of the Type Silicalite-1- α-Alumina
Vlastimil Fíla, Milan Kočiřík, Pavel Hrabánek, Arlette Zikánová, Libor Brabec, Bohumil Bernauer

G4 Measurement and Modeling of Mass Transport in Porous Composite Structures for Adsorption Heat Pumps
Gerrit Füldner

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

…

ADDENDUM

The organizers hope you will have a pleasant time in Athens with many interesting talks and stimulating discussions. We thank you for your participation and would be pleased to welcome you to *Diffusion Fundamentals IV* in New York, USA, in 2011.