

*Final Circular***Diffusion Fundamentals II**
Basic Principles of Theory, Experiment and ApplicationAugust 26th - 29th, 2007
L'Aquila, Italy**Scientific Programme****Sunday, August 26th**

- 15:00 Opening Conference Office
- 17:00 - 17:45 Welcome and Talk of Luca Cavalli-Sforza (Stanford): Genetic and Cultural Diffusion
- 17:45 - 18:30 Entertaining Talk by Albrecht Beutelspacher (Gießen): "(Wo)man on the Street"
- 18:30 - 22:00 Buffet Dinner

Monday, August 27th

- 1st Session** Chairs: Paul Heitjans (Hanover), Roberto Volpe (L'Aquila)
- 09:00 - 09:35 Richard A. Catlow (London): Atomistic Models of Diffusion in Solids
- 09:35 - 10:10 Manfred Martin (Aachen): Diffusion in Oxides
- 10:10 - 10:45 Armin Bunde (Gießen): Percolation and Anomalous Diffusion in Disordered Materials
- 10:45 - 11:45 1st Poster Session and *Coffee Break*
- 2nd Session** Chairs: Alexander V. Neimark (Piscataway), Farida Grinberg (Leipzig)
- 11:45 - 12:20 Nikolaus Nestle (Ludwigshafen): Diffusion Challenges in (Chemical) Industries
- 12:20 - 12:55 Edward L. Cussler (Minneapolis): Diffusion in Self-Assembled Composites
- 12:55 - 13:45 *Lunch break*
- 13:45 - 18:00 Conference Excursion (to *Castelvecchio Calvisio* and *Santo Stefano*)
- 19:00 - 24:00 Conference Dinner ([Casale Signorini](#), [outskirt](#) of L'Aquila)

Tuesday, August 28th

- 1st Session** Chairs: Subramanian Yashonath (Bangalore), Takashi Odagaki (Fukuoka)
- 09:00 - 09:35 Charles Nicholson (New York): Diffusion Reveals Properties of Brain Extracellular Space
- 09:35 - 10:10 Gero Vogl (Wien): The Invasion of Newcomers: Isotopes, Neobiota, Foreigners
- 10:10 - 10:45 Yossi Klafer (Tel Aviv): How Anomalous is Anomalous Diffusion?
- 10:45 - 11:10 *Coffee break*
- 2nd Session** Chairs: Doros N. Theodorou (Athens), Giovanni Del Re (L'Aquila)
- 11:10 - 11:45 Kurt Binder (Mainz): Interdiffusion in Critical Binary Mixtures by Molecular Dynamics Simulation
- 11:45 - 12:20 Dieter Richter (Jülich): Polymer Dynamics: From Synthetic Polymers to Proteins

- 12:20 - 12:55 Giulio Sarti (Bologna): Fickian and non-Fickian Diffusion in Solid Polymers
- 12:55 - 14:00 *Lunch break*
- 14:00 - 16:00 2nd Poster Session and *Coffee Break*

starting from 16:00: option for participating in the L'Aquila festival "Perdonanza"

Wednesday, August 29th

- 1st Session** Chairs: Douglas M. Ruthven (Orono), Nick Kanellopoulos (Athens)
- 09:00 - 09:35 John A. Barker (Southampton): Diffusion in Hydrogeology
- 09:35 - 10:10 Stefano Brandani (Edinburgh): Challenges in Macroscopic Measurement of Diffusion in Zeolites
- 10:10 - 10:45 Hervé Jobic (Villeurbanne): QENS and the Benefit of Diffusion Measurement over Different Length Scales
- 10:45 - 11:45 3rd Poster Session and *Coffee Break*
- 2nd Session** Chairs: Charles Nicholson (New York), William S. Price (Sydney)
- 11:45 - 12:20 Clemens Bechinger (Stuttgart): Diffusion in Reduced Dimensionality
- 12:20 - 12:55 Philip W. Kuchel (Sydney): Diffusion in Cells: NMR Studies
- 12:55 - 13:10 Final Remarks and Closing
- 13:10 - 15:30 *Lunch break* with option for further discussions
- End of the conference*

Location

The conference takes place in the [Castle of L'Aquila](#). The massive 16th-century [Spanish castle](#) crowns the city's highest point and is surrounded by the large Parco del Castello (click for [bird's eye view of the Castle](#) by *Google maps*). Maps indicating the way from your hotel to the Castle can be found on the [accomodation-site](#) (last column *Google maps*, *way to castle*). Information about the local weather can be found at the [CETEMPS-website](#) (University of L'Aquila).

The lecture hall is equipped with overhead projector and laptop (Windows) with beamer.

Excursion

During the conference excursion, two small, lovely villages in the [National Park of Gran Sasso](#) are visited - [Castelvecchio Calvisio](#) and [Santo Stefano di Sessanio](#). The origin of both villages goes back to the Roman Empire. They rose close to the commercial routes between Rome and the Adriatic coast and reached their time of prosperity in the Middle Ages. The appearance at that time could be largely conserved up today.

The busses of the excursion start at 1:45 p.m. at the *Fontana Luminosa* near the Castle. The following [maps](#) (Google maps) shows the way from the entrance of the Castle to *Fontana Luminosa*. After the excursion the buses will stop along a loop close to your hotel and will repeat the loop after 45 minutes to collect us and take us to [Casale Signorini](#), the location of the conference dinner. You will find the details of the bus route in your conference bag.

Posters

All posters can be mounted during the whole conference. The posters are assigned to three different sessions (no flash talks) - on Monday, Tuesday or Wednesday, respectively. A list of all posters can be downloaded [here](#) (pdf, 0.7MB).

A preferable poster size is A0 in upright format, i.e. height x width: 1.19m x 0.84m (47 in x 33 in). In any case, the poster width should not exceed 1 m. Pinning material will be provided.

Authors of contributions which were accepted as posters of the conference are invited to send full papers before September 17th (prolonged). Please follow the instructions given under <http://diffusion.uni-leipzig.de/pdf/layout-full-paper-contribution.doc> and send your paper to tomas@uni-leipzig.de. The publication in the special issue of the Online-Journal "[Diffusion Fundamentals](#)" depends on the positive response of the referees.

Conference Chairmen: [Stefano Brandani](#), London/Edinburgh; [Jörg Kärger](#), Leipzig; [Roberto Volpe](#), L'Aquila

Scientific Committee:

Dezső 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
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Michael J. Saxton, Davis	Gunter Schütz, Jülich	Doros Theodorou, Athens
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Diffusion Fundamentals II

Basic Principles of Theory, Experiment and Application

$$\langle x^2(t) \rangle = 2Dt$$
$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

List of Posters

August 26th to 29th, 2007 – L'Aquila, Italy



POSTER PRESENTATIONS

Poster Presentation I: Monday, August 27th, 10:45 – 11:45

A – Solids

- A1 Anomalous Diffusion on the Nanoscale in Binary Alloys
Zoltán Erdélyi, Dezső L. Beke
- A2 Kinetics of Bulk Nano-Clustering in Silver-Doped Glasses during Reactive Hydrogen Diffusion
Yu. Kaganovskii, A.A. Lipovskii, E. Mogilko, V. Zhurikhina, M. Rosenbluh
- A3 Lateral Diffusion Spreading of Two Competitive Intermetallic Phases along Free Surface (System Cu-Sn)
Yu. Kaganovskii, L.N. Paritskaya, V.V. Bogdanov
- A4 Re-Orientation Behaviour of c-Variant FePt Thin Films
Marcus Rennhofer, Bogdan Sepiol, Gero Vogl, Mirosław Kozłowski, Rafal Kozubski, Bart Laenens, André Vantomme, Johan Meersschaut
- A5 Quasielastic Neutron Scattering Study of Hydrogen Diffusion in C14-Type ZrMn₂H₃
Alexander Skripov, Terrence Udovic, John Rush
- A6 Near Equilibrium in Dissociative Diffusion of Nickel in Silicon
Masayuki Yoshida, Hajime Kitagawa, Masami Morooka, Shuji Tanaka
- A8 Time-Dependent Competition Effects in Diffusion-Limited Crystal Growth
Sergey D. Traytak

B – Theory and Modelling (part I)

- B1 Molecular Dynamics Study of Carbon Diffusion in Cementite
Alexander V. Evteev, Elena V. Levchenko, Irina V. Belova, Graeme E. Murch
- B2 Carbon Diffusion in Austenite: Computer Simulation and Theoretical Analysis
Alexander V. Evteev, Elena V. Levchenko, Irina V. Belova, Graeme E. Murch
- B3 Analytical and Kinetic Monte-Carlo Study Shrinkage by Vacancy Diffusion of Hollow Nanospheres and Nanotubes
Alexander V. Evteev, Elena V. Levchenko, Irina V. Belova, Graeme E. Murch
- B4 Formation of a Surface-Sandwich Structure in Pd-Ni Nanoparticles by Interdiffusion: Atomistic Modelling
Alexander V. Evteev, Elena V. Levchenko, Irina V. Belova, Graeme E. Murch
- B5 Molecular Dynamics Study of Diffusion in Palladium Hollow Nanospheres and Nanotubes
Alexander V. Evteev, Elena V. Levchenko, Irina V. Belova, Graeme E. Murch
- B6 The Effect of the Dislocation Elasticity on the Thermal Motion of Attached Particle
Sergei Prokofjev, Victor Zhilin, Erik Johnson, Ulrich Dahmen



Poster Presentation II: Tuesday, August 28th, 14:00 – 16:00

B – Theory and Modelling (part II)

- B7 Cellular Automata Modeling of Diffusion under Confinement
Pierfranco Demontis, Federico G. Pazzona, Giuseppe B. Suffritti
- B8 Driven Polymer Translocation through a Nanopore: a Manifestation of Anomalous Diffusion
Johan Dubbeldam, Andrey Milchev, Vakhtang Rostiashvili, Thomas Vilgis
- B9 Effects of Superspreaders in Spread of Epidemic
Ryo Fujie, Takashi Odagaki
- B10 Residence Times of Reflected Brownian Motion
Denis S. Grebenkov
- B11 Surface Resistance to Heat and Mass Transfer in a Silicalite Membrane.
A Non-Equilibrium Molecular Dynamics Study.
Isabella Inzoli, Jean Marc Simon, Signe Kjelstrup
- B12 Irreversible $A + B \rightarrow 0$ Reaction – Diffusion Process with Initially Separated Reactants:
Exponential Temporal Asymptotics
Slava Kisilevich, Misha Sinder, Joshua Pelleg, Vladimir Sokolovsky
- B13 Kinetic Monte Carlo Study of Binary Diffusion in MFI-type zeolite
Nicolas Laloué, Catherine Laroche, Hervé Jobic, Alain Méthivier
- B14 Diffusion of Water Molecules in Narrow Carbon Nanotubes and Nanorings
Biswaroop Mukherjee, Prabal K. Maiti, Chandan Dasgupta, A. K. Sood
- B15 Diffusion of *n*-Pentane in Zeolite ZK5
Oraphan Saengsawang, Andreas Schüring, Ton Dammers, David Newsome, Siegfried Fritzsche
- B16 The Probability that a Molecule Enters a Porous Crystal
Andreas Schüring
- B17 Transport in the Transition Region Gas/Adsorbent Studied by Molecular Dynamics Simulations
A. Schüring, J. Gulín-González, S. Fritzsche, J. Kärger, S. Vasenkov
- B18 Size Dependence of Solute Diffusivity and Stokes-Einstein Relationship:
Effect of van der Waals Interaction
Manju Sharma, S. Yashonath
- B19 Adsorption Kinetics of Mixtures of *n*-Hexane and 2-Methylpentane on Silicalite by
Nonequilibrium Molecular Dynamics.
Jean-Marc Simon, Jean-Pierre Bellat
- B20 Dynamical Behaviour of H₂ Molecules on Graphite Surface. A Molecular Dynamics Study
Jean-Marc Simon, Ole-Erich Haas, Signe Kjelstrup, Astrid Lund Ramstad
- B24 Diffusional Atomic-Ordering Kinetics of Close-Packed Solid Solutions:
Models for L1₂ and DO₁₉ Phases
Taras Radchenko, Valentyn Tatarenko, Hélène Zapolsky
- B26 Method of Fractional Derivatives in Time-Dependent Diffusion
Sergey D. Traytak, Tatyana V. Traytak



C – Holes and Channels (part I)

- C1 Diffusion as a Basis for the Determination of Physicochemical Quantities by RF-IGC
T. Agelakopoulou, I. Bassiotis, S. Margariti, B. Siokos, E. Metaxa, F. Roubani-Kalantzopoulou
- C2 Diffusion of Rarified Gases in Silicon Nanotubes
Daniel Albrecht, Alexey Khokhlov, Rustem Valiullin, Jürgen Caro, Jörg Kärger
- C3 Understanding Water Diffusion in Concrete and Clays
Heloisa N. Bordallo, Laurence P. Aldridge, G. Jock Churchman, Will P. Gates, Arnaud Desmedt, Mark T.F Telling
- C4 Diffusion Study of Multi-Component Gas Adsorption in MSC5A by Chromatographic Method
Kazuyuki Chihara, Hidenori Nakamura, Yosuke Kaneko
- C5 Diffusion Measurement of Chlorinated Hydrocarbons into High-Silica Zeolite by Chromatographic Method
Kazuyuki Chihara, Kenta Saito, Hidenori Nakamura, Yosuke Kaneko
- C6 Nuclear Magnetic Resonance Studies of Time Dependent Diffusion in Partially Filled Pores
Germán Farrher, Ioan Ardelean, Rainer Kimmich
- C7 Dynamics of Water in Zeolite NaY(Br) Investigated by NMR
S.A. Lusceac, H. Pahlke, M. Scheuermann, A. Gädke, A. Privalov, F. Fujara
- C8 Adsorption Hysteresis Phenomena in Mesopores
Sergej Naumov, Rustem Valiullin, Jörg Kärger
- C9 Competitive Sorption of Toluene and Acetone on H-ZSM5 Zeolite: Comparison between Molecular Simulation Calculation and Experimental Results
E. Semprini, P. Cafarelli, A. De Stefanis, A.A.G. Tomlinson
- C10 Interference Microscopy Highlights Properties and Peculiarities of SAPO STA-7 Crystals
D. Tzoulaki, M.J. Castro, J. Kärger, P.A. Wright
- C11 NMR Studies on Silica Monoliths - Diffusion in a Hierarchical Pore Structure
M. Wehring, J. Smått, M. Lindén, F. Stallmach, J. Kärger
- C12 Effects of Nanoscale Confinement on Diffusion in Thin Polymer Films
John Torkelson



Poster Presentation III: Wednesday, August 29th, 10:45 – 11:45

C – Holes and Channels (part II)

- C13 Exploring the Diffusion Properties of Pseudomorphic MCM-41 Materials by PFG NMR
Ziad Adem, Flavien Guenneau, Marie-Anne Springuel-Huet, Antoine Gédéon
- C14 Loading Dependence of Diffusion in Zeolites: Combined Benefits of Microscopic Measuring Techniques and Theoretical Approaches
Christian Chmelik, Lars Heinke, Arati Varma, Dhananjai B. Shah, Jörg Kärger, Rajamani Krishna
- C15 Mixture Diffusion in Silicalite-1 Studied by MAS PFG NMR
Moisés Fernandez, André Pampel, Jörg Kärger, Dieter Freude, Jasper M. van Baten, R. Krishna
- C16 The Options of Interference Microscopy to Explore the Significance of Intracrystalline Diffusion and Surface Permeation for Overall Mass Transfer on Nanoporous Materials
Lars Heinke, Pavel Kortunov, Despina Tzoulaki, Jörg Kärger
- C17 Towards Observation of Single-File Diffusion Using TZLC
Abduljelil Ilyas, Mladen Eić, M. Hassan Zahedi-Niaki, Sergey Vasenkov
- C18 Exploring the Influence of Surface Resistance of Nanoporous Particles on the Molecular Transport by PFG NMR
Margarita Krutyeva, Jörg Kärger, Sergey Vasenkov
- C19 Mesopore Functionalization as Highly Specific Tool for the Control of Single Molecule Dynamics in Silica Materials
Timo Lebold, Julia Blechinger, Lea Mühlstein, Christophe Jung, Johanna Kirstein, Thomas Bein, Klaus Müllen, Christoph Bräuchle
- C20 ¹H NMR Signal Broadening in Spectra of MFI Type Zeolites
Ekaterina Romanova, Bärbel C. Krause, Alexander Stepanov, Jasper M. van Baten, R. Krishna, Jörg Kärger, Dieter Freude

D – Fluids and Soft Matter: From (Bio-)Molecules to Man

- D1 Diffusion in Silicate Melts: Kinetics and Mechanisms of Redox Reactions
B. Cochain, V. Magnien, D.R. Neuville, P. Richet
- D2 Intermittent Brownian Dynamics over Strands
P. Levitz
- D3 Tracer Diffusion in HEMA Based Polymer Hydrogels
Jan Pilař, Jaroslav Kříž, Bohumil Meissner
- D4 Dynamic Crossover in Polymers, Role of Molecular Weight
Sebastian Pawlus, Yoshi Hayashi, Kunal Kumar, Alexei P. Sokolov
- D5 No Indications of Fragile-to-Strong Transition in Water of Protein Hydration
Sebastian Pawlus, Sheila Khodadadi, Alexei P. Sokolov
- D6 Anisotropic Diffusion of Flexible Random-Coil Polymers Measured in Brain Extracellular Space by Integrative Optical Imaging
Fanrong Xiao, Charles Nicholson, Sabina Hrabetova



E – Power of Experiment

- E1 A Web Site Dedicated to Materials Science Education, Specially Diffusion
Daniel Monceau, Jean Philibert
- E2 Methodical Aspects of 2D NMR Correlation Spectroscopy under Conditions of Ultra High Pulsed Field Gradients
Marcel Gratz, Petrik Galvosas
- E3 Combined Use of Pulsed Gradient Spin Echo and High Resolution Magic Angle Spinning to Investigate Solutes Diffusion in Presence of a Chromatographic Stationary Phase
Stéphane Viel, Grégory Excoffier, Guilhem Pagès, Fabio Ziarelli, Corinne Delaurent, Stefano Caldarelli

F – Last Minutes' Posters *

Poster Session

- F1 One-step Hydrocarbons Steam Reforming and CO₂ Capture
Luca Di Felice, Claire Courson, Katia Gallucci, Nader Jand, Sergio Rapagnà, Pier Ugo Foscolo and Alain Kiennemann II
- F2 The Glass Transition near the Free Surface
Marcin Sikorski, Christian Gutt, Frank-Uwe Dill, Hermann Franz III
- F3 Characterizing Colloidal Nanocrystals with NMR looking at the Capping Ligand
Bernd Fritzingler, Iwan Moreels, Petra Lommens, Zeger Hens and José C. Martins III
- F4 SEM Analysis Application to Study CO₂ Capture by Means of Dolomite
Katia Gallucci, Ferdinando Paolini, Luca Di Felice, Claire Courson, Pier Ugo Foscolo and Alain Kiennemann II
- F5 Surface Self Diffusion of Hydrogen on Carbon Support by Quasielastic Neutron Scattering
Ole-Erich Haas, Signe Kjelstrup, Astrid Lund Ramstad, Peter Fouquet, Stéphane Rols and Hannu Mutka I
- F6 Hydrodynamic Dispersion in Pressure-Driven and Electroosmotic Flows Probed by Nuclear Magnetic Resonance Techniques
Yujie Li, German Farrherr, Rainer Kimmich II
- F7 Transport Properties of Nanoparticles Studied by Brownian Dynamics Simulations
Tom R. Evensen, Stine N. Naess and Arnljot Elgsaeter I
- F8 Normal and Anomalous Knudsen Diffusion in 2D and 3D Channel Pores
Stephan Zschiegner, Stefanie Russ, Armin Bunde and Jörg Kärger II
- F9 Autocatalytic Reaction-Diffusion Processes in Restricted Geometries
Elena Agliari, Raffaella Burioni, Davide Cassi, Franco M. Neri I
- F10 Electrophoretic NMR (eNMR) – Methods and Applications
Fredrik Hallberg, Erik Pettersson, Sergey Dvinskikh, Thomas Vernersson, Göran Lindberg, István Furó and Peter Stilbs III
- F11 Translational Dynamics of Hemoglobin in Crowded Solutions by PGSE and OGSE NMR
Chris J. Garvey and Philip W. Kuchel III
- F12 A Pure Prediction Model for Penetrant Molecular Diffusivity in Polymer Systems
Hidenori OHASHI, Taichi ITO and Takeo YAMAGUCHI III



F – Last Minutes' Posters*, continued

Poster Session

F13 Red Blood Cell Shape Evolution Probed by Fast-Diffusion Nuclear Magnetic Resonance Measurements <i>Guilhem Pages and Philip W Kuchel</i>	III
F14 Determination of Transport Properties of Gadolinia Doped Ceria Powders from SIMS Profiles <i>Sathya Swaroop, Martin Kilo and Ilan Riess</i>	I
F15 Effects of Polydispersity on PGSE NMR Coherence Features <i>Nirbhay N. Yadav and William S. Price</i>	III
F16 NMR Characterization of Dispersant-Particle Interactions in the Colloidal Dispersions <i>Agnieszka Szczygiel, Leo Timmermans and José C. Martins</i>	III
F17 Diffusion of Hydrocarbons in Zeolites and other Molecular Sieves by ZLC <i>Celio L. Cavalcante Jr. and Diana C. S. Azevedo</i>	III
F18 Adsorption Kinetics of Chlorinated Hydrocarbons into High Silica Zeolite <i>Kazuyuki Chihara, Shinji Kondo and Takashi Matsumoto</i>	III
F19 Textbook: Diffusion in Solids <i>Helmut Mehrer</i>	I
F20 The Effectiveness of Dolomite and Ni-Catalyst Mixture for pure H ₂ Production by Methane Steam Reforming via CO ₂ Capture <i>Nurgul Seitkaliyeva, Nader Jand and Pier Ugo Foscolo</i>	I
F21 Some Considerations about the Modelling of Single File Diffusion <i>Giuseppe B. Suffritti, Alessandro Taloni and Pierfranco Demontis</i>	I

* Some of the last minutes' posters are selected for presentation in poster sessions I or II.