

# Diffusion Fundamentals



August 21-24, 2011

Center for Biotechnology and Interdisciplinary Studies

Rensselaer Polytechnic Institute

Troy, NY

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The Center for Biotechnology and Interdisciplinary Studies is a 218,000-square-foot facility that contains laboratories for molecular biology, analytical biochemistry, microbiology, imaging, histology, tissue and cell culture, proteomics, and scientific computing and visualization.

# Diffusion Fundamentals

## Basic Principles of Theory, Experiment and Application

Dear Participants:

Welcome to the *Diffusion Fundamentals IV* International Conference!

We hope that you will enjoy this multidisciplinary scientific conference, held for the first time outside Europe, after exciting meetings in Leipzig, Germany (2005), L'Aquila, Italy (2007) and Athens, Greece (2009). It all started with the memorable celebration in Leipzig organized by Jörg Kärger, Farida Grinberg, and Paul Heitjans for the 150<sup>th</sup> anniversary of Adolf Fick's *Über Diffusion* (1855) and 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 program once more testifies of the breadth and importance of diffusion as a physical phenomenon, with ramifications to fields as seemingly distant as medicine and the geosciences, but with common roots in physics, and strong connections to chemical engineering and materials science. For a phenomenon that has been investigated for so long, and is associated to the names of legendary scientists, it is remarkable how much *fundamental* progress has still been made over these past few years. This is in part driven by *applications*, in part thanks to the ability to synthesize nanoporous materials of well-controlled structure, and, crucially, thanks to rapid advances in experimental characterization and computational methods that are responsible for fundamental insights and applications that were unthinkable only a few years ago. Diffusion is once again "hot," and moving quickly in all directions!

Oral presentations, by leading scientists in the field, will highlight recent developments, linked by their underlying physics, albeit not in a trivial manner and with distinctive flavors. They are grouped under seven themes:

- *Diffusion in the Brain* (Sunday afternoon)
- *Diffusion in Physiology and Medicine* (Monday morning)
- *Transport Phenomena in Nano-Biotechnology* (Monday morning)
- *Membrane Diffusion Fundamentals - Experiments and Theory* (Monday afternoon)
- *Diffusion in Nanomaterials - Synthesis, Characterization and Applications* (Monday afternoon and Wednesday morning)
- *Theoretical Fundamentals of Confinement Effects on Diffusion* (Monday afternoon and Tuesday morning)
- *Transport in the Geosciences* (Tuesday morning)

No less important are the poster sessions, which can be enjoyed over lunch or coffee, and will remain on view from Monday until Wednesday. Excellent abstracts promise to show us the newest directions in the field.

During your time here, we also hope that you will enjoy the beautiful campus of Rensselaer Polytechnic Institute, founded in 1824 and the oldest engineering school in the English-speaking world, as well as some of its nearby world-class natural and cultural attractions. While our scientific program will keep you engaged, we wanted to ensure that you have an opportunity to relax and enjoy some of the sights, during the excursion to the Berkshires on Tuesday afternoon, and the Curtis R. Priem Experimental Media and Performing Arts Center (EMPAC) at Rensselaer on Monday evening.

Last but not least, we are very grateful to our distinguished speakers and chairmen to accept our invitation, and our poster presenters for showing their newest research.

A conference like this would not be possible without generous support – in funds, time and effort. Our heartfelt thanks go to the U.S. National Science Foundation (NSF-CBET) and the Rensselaer Vollmer Fries Distinguished Lectures for exceptional financial support. Air Products, ExxonMobil Research and Engineering, Fonds der Chemischen Industrie, Praxair, Quantachrome Instruments, Schlumberger, and Süd-Chemie are most gratefully acknowledged for their sponsorship, even during economically challenging times. Without them, this event would be impossible.

Rensselaer's Provost, Dr. Robert Palazzo, and his office have been especially supportive and effective in organizational aspects, engaging the university's Division of Strategic Communications and External Relations – we are very grateful to Trish Galvin, Cheryl McGlothlin, and Michael Mullaney for devoting considerable time and effort. It has been a great pleasure working with them. We thank the office of the Rensselaer Vice President for Research (Wolf von Maltzahn, Jack Huang) for guidance and support. All of you have been in contact with Elaine Belokopitsky, who has been of great help in all matters related to financial administration. Our gratitude also goes to Sharon Sorell and Phylis Federici. A special word of thanks goes to Rose Primett, an administrator in the Department of Chemical and Biological Engineering, who made countless phone calls and arrangements for catering, accommodation, and events.

Overall, we trust that the multidisciplinary character of the meeting, its scientific and social events, will stimulate novel ideas and random walks to beautiful and unexpected collaborations.

We wish you an exciting conference!

Marc-Olivier Coppens, *Rensselaer Polytechnic Institute*  
Alex Neimark, *Rutgers University*  
Douglas Ruthven, *University of Maine*  
Matthias Thommes, *Quantachrome Instruments*

# Diffusion Fundamentals

August 21<sup>st</sup>- 24<sup>th</sup>, Rensselaer Polytechnic Institute, Troy, NY, USA

## Conference Chairs

Marc-Olivier Coppens, Rensselaer Polytechnic Institute, Troy, NY  
Alexander V. Neimark, Rutgers University, New Brunswick, NJ  
Douglas M. Ruthven, University of Maine, Orono, ME  
Matthias Thommes, Quantachrome Instruments, Boynton Beach, FL

## Honorary Chairs

Jörg Kärger, University of Leipzig, Leipzig, Germany

## Session Chairs

Edward (Ned) Corcoran, ExxonMobil Research  
Mladen Eic, University of New Brunswick  
Keith Gubbins, North Carolina State University

Nick Kanellopoulos, NCSR Demokritos, Athens  
Jörg Kärger, University of Leipzig  
William Price, University of Western Sydney

## Opening Lecture

James Wei, Princeton University

## Invited Speakers

Joe Ackerman, Washington Univ.  
Bernhard Blümich, RWTH Aachen  
Thomas Franosch, TU Munich

Pierre Levitz, Ecole Polytechnique  
Murugappan Muthukumar,  
UMass Amherst

Yunfeng Shi, Rensselaer  
Rustem Valiullin, Leipzig Univ.  
Andrew Zydney, Penn State Univ.

James Baish, Bucknell Univ.  
Frank Cichos, Leipzig Univ.  
Sabina Hrabetova,  
SUNY Downstate  
Don MacElroy, Univ Coll Dublin  
Peter Pfeifer, Univ. Missouri  
Columbia  
Tom Truskett, UT Austin  
Sergey Vasenkov, Univ. Florida

Georges Belfort, Rensselaer  
Jens Feder, Univ. Oslo  
John Kasianowicz,  
NIST, Gaithersburg  
Peter Monson, UMass Amherst  
Joel Plawsky, Rensselaer

Theo Tsotsis, Univ. Southern California  
Bruce Watson, Rensselaer

## Local Organizing Committee (RPI)

Elaine Belokopitsky  
Trish Galvin  
Rosemary Primett

Marc-Olivier Coppens  
Cheryl McGlothlin  
Sharon Sorell

Phylis Federici  
Michael Mullaney

## Scientific Committee

Dezsö L. Beke, Debrecen  
Paul Callaghan, New Zealand  
Marc-Olivier Coppens, Troy  
Dieter Freude, Leipzig  
Jörg Kärger, Leipzig  
Alfred Leipertz, Erlangen-Nuremberg  
Jean Philibert, Paris  
Michael J. Saxton, Davis  
Rustem Valiullin, Leipzig  
George H. Weiss, Bethesda

Stefano Brandani, Edinburgh  
Alan Chadwick, Canterbury  
Mladen Eic, Frederickton  
Farida Grinberg, Jülich  
Yossi Klafter, Tel Aviv  
Andreas Mandelis, Toronto  
William S. Price, Sydney  
Gunter Schütz, Jülich  
Ilpo Vattulainen, Helsinki

Armin Bunde, Giessen  
Christian Chmelik, Leipzig  
Gerhard Ertl, Berlin  
Paul Heitjans, Hannover  
Klaus Kroy, Leipzig  
Graeme Murch, Callaghan  
Douglas M. Ruthven, Orono  
Doros Theodorou, Athens  
Gero Vogl, Vienna

# Diffusion Fundamentals IV

August 21-24, 2011, Rensselaer Polytechnic Institute, Troy, NY

*All lectures are in the Rensselaer Center for Biotechnology and Interdisciplinary Studies (CBIS).  
All posters remain on display in the CBIS Atrium, Monday-Wednesday for continuous viewing.*

*Each day there will be shuttle buses between the Hilton Garden Inn, Troy, N.Y., and CBIS in the morning, from 7-9 am.  
There will also be shuttle buses after the last scientific event of the day, except for Monday, when the Shuttle will travel to the dinner location in Troy and return to the Hilton later in the evening.*

## Sunday, 21 August

2:30-3:15 p.m. Shuttle bus from Hilton Garden Inn, Troy, NY, to CBIS, Rensselaer

3:15 Welcoming message by Marc-Olivier Coppens – CBIS Auditorium

### **Rensselaer Vollmer Fries Distinguished Lecture**

(Chair: Jörg Kärger, *University of Leipzig*)

3:30 p.m. **James Wei**, *Princeton University*, “Diffusion in tight mazes”

### **Session 1: Diffusion in the Brain**

(Chair: Charles Nicholson, *New York University*)

4:30 p.m. Joseph Ackerman, *Washington University in St. Louis*, “Diffusion sensitive MR in biological systems: Insights, puzzles, pitfalls”

5:05 Sabina Hrabetova, *SUNY Downstate Medical Center*, “Extracellular diffusion in brain: Distinct diffusion regimes at different spatial scales”

5:40 *Session 1 close*

6:00 *Welcoming reception and dinner – Hilton Garden Inn*

## Monday, 22 August

### **Session 2: Diffusion in Physiology and Medicine**

(Chair: William Price, *University of Western Sydney*)

8:45 a.m. James Baish, *Bucknell University*, “Diffusion in tumors and normal tissues”

9:20 Peter Pfeifer, *University of Missouri, Columbia*, “Diffusion-reaction in space-filling networks: oxygen transport in the lung”

10:05 *Session 2 close*

10:05-10:30 *Coffee break*

**Poster presenters:** *Please hang posters (CBIS Atrium)*

### **Session 3: Transport Phenomena in Nano-Biotechnology**

(Chair: Alex Neimark, *Rutgers University*)

10:30 a.m. Murugappan Muthukumar, *University of Massachusetts, Amherst*, “Macromolecular transport through nanopores”

11:05 John Kasianowicz, *National Institute for Science and Technology, Gaithersburg*, “Single molecule transport in nanometer-scale pores: A tool for polymer science and practical applications”

11:40 *Session 3 close*

11:40-2:10 p.m. *Lunch buffet (Bruggeman Conference Center, CBIS)*

#### **POSTER SESSION 1 (CBIS Atrium)**

#### **Session 4: Membrane Diffusion Fundamentals - Experiments and Theory**

(Chair: Douglas Ruthven, *University of Maine*)

2:10 p.m. Georges Belfort, *Rensselaer Polytechnic Institute*, “Diffusion in synthetic and natural membranes: Critical for success”

2:45 Andrew Zydney, *Pennsylvania State University*, “Diffusional contributions and electrostatic exclusion effects on transport through ultrafiltration membranes”

3:20 *Session 4 close*

#### **Session 5: Diffusion in Nanomaterials: Synthesis, Characterization and Applications, I**

(Chair: Mladen Eic, *University of New Brunswick*)

3:20 p.m. Theo Tsotsis, *University of Southern California*, “Preparation, characterization, and modeling of nanoporous silicon carbide membranes”

3:55 Rustem Valiullin, *University of Leipzig*, “Diffusion of fluids in mesoporous host materials”

4:30 *Session 5 close*

4:30-5:00 *Tea break*

#### **Session 6: Theoretical Fundamentals of Confinement Effects on Diffusion, I**

(Chair: Matthias Thommes, *Quantachrome Instruments*)

5:00 p.m. Tom Truskett, *University of Texas at Austin*, “Entropy scaling, structure, and dynamics of confined fluids”

5:35 Peter Monson, *University of Massachusetts, Amherst*, “Dynamic mean field theory for fluids in mesoporous materials”

6:10 Yunfeng Shi, *Rensselaer Polytechnic Institute*, “Molecular simulations on gas diffusion in nanoporous carbon”

6:45 *Session 6 close*

7:00 *Tour of Curtis R. Priem Experimental Media and Performing Arts Center (EMPAC)*

8:00 *Dinner Event*

### **Tuesday, 23 August**

#### **Session 7: Theoretical Fundamentals of Confinement Effects on Diffusion, II**

(Chair: Keith Gubbins, *North Carolina State University*)

8:15 a.m. Joel L. Plawsky, *Rensselaer Polytechnic Institute*, “Drift, diffusion and dielectric breakdown”

8:50 Pierre Levitz, *Ecole Polytechnique, Paris*, “Molecular intermittent dynamics in interfacial confinement”

9:25 Thomas Franosch, *University of Erlangen-Nürnberg*, “Complex transport in strongly disordered materials”

10:00            *Session 7 close*  
10:00-10:15    *Coffee break*

### **Session 8: Transport in the Geosciences**

(Chair: Edward Corcoran, *ExxonMobil Research*)

10:15 a.m.        E. Bruce Watson, *Rensselaer Polytechnic Institute*, “Diffusion in solid-Earth systems”  
10:50            Jens Feder, *University of Oslo, Norway*, “Diffusion, dissolution and dispersion”  
11:25            *Session 8 close*  
11:30-1:30 p.m. *Lunch (Russell Sage Dining Hall) –*

### **POSTER SESSION 2 (CBIS Atrium)**

*Shuttle bus available between CBIS, Rensselaer and Hilton Garden Inn, Troy*

1:30 p.m.        (**sharp!**) Departure by Yankee Trails bus, from CBIS, for excursion

1:30-10:00 p.m. *Excursion to the Berkshires, along the Mohawk Trail.*  
*Visit to MASS MoCA in North Adams, MA, followed by dinner, and a short walk in Williamstown, MA. Musical theatre production of Ten Cents a Dance at Williamstown Theatre Festival in Williamstown, MA.*

## **Wednesday, 24 August**

### **Session 9: Diffusion in Nanomaterials: Synthesis, Characterization and Applications, II**

(Chair: Nick Kanellopoulos, *NCSR Demokritos, Athens*)

8:45 a.m.        Bernhard Blümich, *RWTH Aachen*, “Diffusion and relaxation probed by mobile NMR”  
9:20            Don MacElroy, *University College Dublin*, “Molecular simulation of the fabrication and permselective characterisation of thin nanoporous silica films”  
9:55            Sergey Vasenkov, *University of Florida*, “Structure-transport relationship in organized soft matter systems by diffusion NMR”  
10:30            *Session 9 close*  
10:30-11:50    *Coffee break*

### **POSTER SESSION 3 (CBIS Atrium)**

### **Rensselaer Vollmer Fries Distinguished Lecture**

11:50 a.m.        Frank Cichos, *University of Leipzig*, “From hot Brownian motion to self-propelled particles,” and introduction to *Diffusion Fundamentals V*  
12:25 p.m.        Closing remarks: Marc-Olivier Coppens, *Rensselaer Polytechnic Institute*  
12:30            *Conference closes*  
12:30-1:30        *Lunch buffet (Bruggeman Conference Center, CBIS)*  
**Poster presenters: Please remove posters**

## Poster Presentations

### A. Diffusion in Biology, Physiology and Medicine

No.	Authors	Affiliation	Title
A5	<i>Florian Feil, Anna Sauer, Jens Michaelis, Thomas Bein, Christoph Bräuchle</i>	LMU München	Single Molecule Diffusion Studies of Mesoporous Materials: From Material Science to Drug-Delivery Applications
A1	<i>Padideh Kamali-Zare &amp; Charles Nicholson</i>	New York University	Monte Carlo Modeling of Molecular Diffusion in Brain Extracellular Space
A2	<i>David P. Lewis, Sabina Hrabetova, Jan Hrabce</i>	Nathan S. Kline Institute for Psychiatric Research	Model of Extracellular Diffusion in Layered Structure of Hippocampus
A3	<i>Charles Nicholson</i>	New York University	Extracellular Diffusion in Oriented Bundles of Brain Fibers with Variable Volume Fraction
A6	<i>Ryan J. Dean, Timothy Stait-Gardner, Simon J. Clarke, Suzy Y. Rogiers, William S. Price</i>	University of Western Sydney	Diffusion Tensor Imaging (DTI) Studies of the Grape Berry
A7	<i>Michael J. Saxton</i>	University of California Davis	Move, Dither, Move, Dither. On the Structure of Random Walks and Single-Particle Trajectories
A4	<i>Fanrong Xiao, Sabina Hrabetova</i>	SUNY Downstate Medical Center	Monte Carlo Simulation Study of Geometrical Factors Causing Anomalous Diffusion in Brain Extracellular Space

## B. Diffusion in Membranes

No.	Authors	Affiliation	Title
B1	<u>Sebastien Balme</u> , <u>Jean-Marc Janot</u> , <u>Philippe Dejardin</u> , <u>Lydie Bérardo</u> , <u>Francois Henn</u> , <u>Daniel Bonhenry</u> , <u>Sebastian Kraszewski</u> , <u>Fabien Picaud</u> and <u>Christophe Ramseyer</u>	Inst. Charles Gerhardt, CNRS, Montpellier	Ionic Diffusion Through a Bio-inspired Membrane
B2	<u>Tianhong Chen</u> , <u>Bjoern Reinhard</u>	Boston University	A Novel Free Standing Lipid Membrane Model Designed for Dark Field Microscopy
B3	<u>George Pilatos</u> , <u>Eleni Vermisoglou</u> , <u>Anastasios Labropoulos</u> , <u>Charitomeni Veziri</u> , <u>George E. Romanos</u> , <u>George N. Karanikolos</u> , <u>Nick K. Kanellopoulos</u>	Demokritos National Research Center, Athens, Greece	Pore Structure Evaluation of Carbon Nanotube and Inorganic Membranes through Sorption and Permeability Studies
B4	<u>Silo Meoto</u> , <u>Marc-Olivier Coppens</u>	Rensselaer Polytechnic Institute	Anodic Alumina-Mesoporous Silica Hybrid Membranes: A Systematic Study Of Alumina Filling
B5	<u>Guoxin Rong</u> , <u>Hongyun Wang</u> , and <u>Björn M. Reinhard</u>	Boston University	Insights from a Nanoparticle Minuet: Two-Dimensional Membrane Profiling through Silver Plasmon Ruler Tracking
B6	<u>Sonia Lequina</u> , <u>Jean-Pierre Bellat</u> , <u>Jean-Marc Simon</u> , <u>Thomas Karboviak</u> , <u>Laurent Brachais</u> , <u>David Chassagne</u>	Université de Bourgogne	Oxygen Diffusion Through Natural Raw Cork
B7	<u>Mingyan Zhou</u> , <u>Ke Wu</u> , <u>James E. Kilduff</u> , <u>Georges Belfort</u>	Rensselaer Polytechnic Institute	Modeling Organic Molecules Transport Through Nanofiltration Membranes

## C. Diffusion in Nanomaterials: Synthesis, Characterization and Applications

No.	Authors	Affiliation	Title
C1	<u>Steffen Beekert</u> , <u>Frank Stallmach</u> , <u>Jens Kullmann</u> , <u>Dirk Enke</u>	University of Leipzig	Concentration Dependent Self-Diffusion Coefficients of Aqueous Electrolyte Solutions in Bulk Phase and Confined in Porous Glasses Measured by Pulsed Field Gradient NMR
C2	<u>Daniel J. Beltran-Villegas</u> , <u>Michael A. Bevan</u>	Johns Hopkins University	A Smoluchowski Model of Colloidal Crystallization Dynamics
C3	<u>P. Bottke</u> , <u>S. Nakhai</u> , <u>M. Lerch</u> , <u>P. Heitjans</u> , <u>M. Wilkening</u>	Leibniz University of Hannover	Revealing Li <sup>+</sup> Exchange in the $\beta$ -modification of Li <sub>3</sub> VF <sub>6</sub> by <sup>6</sup> Li 2D MAS NMR Spectroscopy
C4	<u>Kazuyuki Chihara</u> , <u>Shingo Ito</u> , <u>Hideaki Nagashima</u> , <u>Mai Hikita</u> , and <u>Ryota Suzuki</u>	Meiji University	Adsorption of Organics on MSC5A in Supercritical CO <sub>2</sub> , Chromatographic Measurements & Stop & Go Simulation
C5	<u>Satoshi Nakagawa</u> , <u>Kazuyuki Chihara</u> , <u>Kuniyasu Ogawa</u>	Meiji University	2D Projective Imaging of Water Concentration Profiles in Adsorption Columns by MRI
C6	<u>Carmine D'Agostino</u> , <u>Lynn F. Gladden</u> and <u>Mick D. Mantle</u>	University of Cambridge	Hydrogen Bonding Network Disruption in Nanoporous Catalyst Supports Probed by PFG-NMR Diffusometry and NMR Relaxometry
C7	<u>Muslim Dvoyashkin</u> , <u>Ryan Wood</u> , <u>Clifford R. Bowers</u> , <u>Shreya Mukherjee</u> , <u>George Christou</u> , <u>Ipek Yucelen</u> , <u>Sankar Nair</u> , <u>Aakanksha Katihar</u> , <u>Sergey Vasenkov</u>	University of Florida	Transport through Unidimensional Nanochannels: The Potential of Pulsed Field Gradient and Hyperpolarized Tracer Exchange NMR Spectroscopy
C8	<u>Laurent Gueudré</u> , <u>Christian Chmelik</u> , <u>Jörg Kärger</u>	University of Leipzig	Diffusion Anisotropy in a Single Crystal of Silicalite-1 Studied by Interference Microscopy
C9	<u>Florian Hibbe</u> , <u>Lars Heinke</u> , <u>Christian Chmelik</u> , <u>Sanhita Pramanik</u> , <u>Jing Li</u> , <u>Douglas M. Ruthven</u> , <u>Despina Tzoulaki</u> , <u>Jörg Kärger</u>	University of Leipzig	The Nature of Surface Barriers on Nanoporous Solids Explored by Microimaging of Transient Guest Distributions and Monte Carlo Simulations

No.	Authors	Affiliation	Title
C10	<u>Florian Hibbe</u> , <u>Christian Chmelik</u> , <u>V.R. Reddy Marthala</u> , <u>Jörg Kärger</u> , <u>Jens Weitkamp</u>	University of Leipzig	Diffusion Studies on Large-Crystal Ferrierite Zeolites of Different Chemical Composition and Post-Synthesis Treatment
C11	<u>C. Iacoby</u> , <u>J. R. Sangoro</u> , <u>R. Valiullin</u> , <u>R. Gläser</u> , <u>J. Kärger</u> <u>and F. Kremer</u>	University of Leipzig	Charge Transport in Confined Ionic Liquids
C12	<u>Christian Chmelik</u> , <u>Helge Bux</u> , <u>Jürgen Caro</u> , <u>Lars Heinke</u> , <u>Florian Hibbe</u> , <u>Tobias Titze</u> , <u>Jörg Kärger</u>	University of Leipzig	Faster by Opposing the Stream
C13	<u>W. Kipnusu</u> , <u>C. Iacoby</u> , <u>J. Sangoro</u> and <u>F. Kremer</u>	University of Leipzig	Molecular Dynamics of Tris(2-ethylhexyl)phosphate in 2D Confinement
C14	<u>Daria Kondrashova</u> , <u>Rustem Valiullin</u>	University of Leipzig	Diffusion in Mesoporous Materials During Melting and Freezing
C15	<u>M. Kathryn Lee</u> , <u>S.M. Cundy</u> , <u>David C. Calabro</u> , <u>Quanchang Li</u> , <u>Dennis Peiffer</u>	ExxonMobil Corporate Strategic Research	A New Technique for the Measurement of CO <sub>2</sub> Diffusion in Thin Polymer Films
C16	<u>M. G. Mazza</u> , <u>M. Greschek</u> , <u>R. Valiullin</u> , <u>J. Kärger</u> , <u>M. Schoen</u>	TU Berlin	Dynamics in Reentrant Nematics
C17	<u>Dirk Mehlhorn</u> , <u>Rustem Valiullin</u> , <u>Jörg Kärger</u> , <u>Ryong Ryoo</u>	University of Leipzig	Diffusion in Mesoporous Zeolites
C18	<u>Frank Cichos</u> , <u>Martin Pumpha</u>	University of Leipzig	Single Molecule Diffusion in Liquid Crystals
C19	<u>Shasad Sharif</u> , <u>Lynn DiMemmo</u> , <u>Martha Davidovich</u> , <u>Beth Sarsfield</u>	Bristol-Myers Squibb Company	Applicability of Specific Surface Area Determination on Pharmaceuticals by Inverse Gas Chromatography
C20	<u>Elenica Shiko</u> , <u>John Lowe</u> , <u>Karen Edler</u> , <u>Sean Rigby</u>	University of Bath	Probing Longer-Range Co-operative Effects in Vapour Adsorption and Solid Melting Within Mesoporous Solids using NMR Relaxometry and Cryodiffusometry
C21	<u>Tobias Titze</u> , <u>Christian Chmelik</u>	University of Leipzig	Configurational Entropy and Intersection Blocking Effects in Multi-component Systems in MFI-type Zeolites Studied by IR Microscopy
C22	<u>Sen-Ming Wang</u> , <u>Rohit Kanungo</u> , <u>Bendaoud Nohair</u> , <u>Sergey Vasenkov</u> , <u>Serge Kaliaguine</u>	Laval University, Québec	Self-Diffusion of Methyl Oleate in Mesoporous Materials with SBA-16 Structure

No.	Authors	Affiliation	Title
C23	<u>Markus Wehring</u> , <u>Saeed Amirjalayer</u> , <u>Rochus Schmid</u> , <u>Frank Stallmach</u>	University of Leipzig	Anisotropic Self-Diffusion of Guest Molecules in Zn <sub>2</sub> (bdc) <sub>2</sub> dabco
C24	<u>Patrick C. With</u> , <u>S. Fichtner</u> , <u>B. Böhrringer</u> , <u>M. Lutecki</u> , <u>S.</u> <u>Naumov</u> , <u>R. Valiullin</u> , <u>R. Gläser</u>	University of Leipzig	Diffusion in Hierarchically Structured Zirconia Spheres
C25	<u>Masayuki Yoshida</u> , <u>Satoru Matsumoto</u> , <u>Shuji Tanaka</u>	Yoshida Semiconductor Laboratory	Application of Watkins' Model of Phosphorus- and Arsenic-Vacancy Pairs to the Interstitial-Diffusion of Phosphorus and Arsenic in Silicon
C26	<u>Philipp Zeigermann</u> , <u>Muslim Dvoyashkin</u> , <u>Roger Gläser</u> and <u>Rustem Valiullin</u>	University of Leipzig	Self-Diffusion in Mesoporous Solids at Sub- and Supercritical Conditions

## D. Theoretical Fundamentals of Confinement Effects on Diffusion

No.	Authors	Affiliation	Title
D1	<u>Tomas Binder</u> , <u>Christian Chmelik</u> , <u>Jörg Kärger</u> , <u>Wolfgang Schmidt</u>	University of Leipzig	Microscopic Analysis of Phase Transition Effects during Benzene Sorption in MFI Type Zeolites
D2	<u>Qu Chen</u> , <u>Yingchun Liu</u> , <u>Qi Wang</u> , <u>Keith E. Gubbins</u>	Zhejiang University	The Role of Hydrogen Bond in Mechanism of Water Diffusion in Carbon Nanotubes
D3	<u>Meng Miao</u> , <u>Yingchun Liu</u> , <u>Tao Wu</u> , <u>Qi Wang</u> , <u>Keith E. Gubbins</u>	Zhejiang University	Does a Hydrogen Atom/Proton Diffuse Through Graphene ?
D4	<u>Jeffrey A. Marquis</u> , <u>Marc-Olivier Coppens</u>	Rensselaer Polytechnic Institute	Enhanced Performance of Low Temperature PEM Fuel Cells by Introducing Hierarchically Structured Macroporosity to the Cathode Catalyst Layer
D5	<u>Mikuláš Peksa</u> , <u>Jan Lang</u> , <u>Milan Kočirik</u>	Charles University in Prague	Hexane Self-Diffusion in Bed of Glass Spheres. Testing Applicability Range of the Pore-Hopping Model
D6	<u>Benjamin F. Moroney</u> , <u>Timothy Stait-Gardner</u> , <u>Gang Zheng</u> , <u>William S. Price</u>	University of Western Sydney	Numerical Analysis of NMR Diffusion Experiments in Complex Systems
D7	<u>Sanjeev M. Rao</u> , <u>Marc-Olivier Coppens</u>	Rensselaer Polytechnic Institute	Increasing Robustness of Deactivating Nanoporous Catalysts by Optimizing the Pore Network—Application to Hydrodemetalation
D8	<u>Joshua Sangoro</u> , <u>Ciprian Iacob</u> , <u>Rustem Valiullin</u> , <u>Jörg Kärger</u> and <u>Friedrich Kremer</u>	University of Leipzig	Diffusion in Ionic Liquids: The Interplay Between Molecular Structure and Dynamics
D9	<u>Sondre K. Schnell</u> , <u>Thijs J.H. Vlugt</u> , <u>Jean-Marc Simon</u> , <u>Signe Kjølstrup</u> , <u>Dick Bedeaux</u>	Université de Bourgogne	Direct Calculation of the Thermodynamic Correction Factor, Gamma, from Molecular Dynamics Simulations
D10	<u>Jean-Marc Simon</u> , <u>Nicole Floquet</u> , <u>Jean-Pierre Bellat</u> , <u>Guy Weber</u>	Université de Bourgogne	Commensurate Diffusion Effects of n-Heptane in Silicalite-1
D11	<u>Thijs J.H. Vlugt</u> , <u>Xin Liu</u> , <u>André Bardow</u>	Delft University of Technology	Multicomponent Maxwell-Stefan Diffusivities at Infinite Dilution
D12	<u>Scott A. Willis</u> , <u>Gary R. Dennis</u> , <u>Gang Zheng</u> , <u>William S. Price</u>	University of Western Sydney	Self-Diffusion of Water in Compressed Hexagonal Phases: Experimental and Simulated Results
D13	<u>Frerich J. Keil</u> , <u>Nils E. R. Zimmermann</u>	Hamburg University of Technology	Transport Barriers as Triggered by the Idealized Microscopic Crystal Surface and the Role of the Evaluation Protocol of Diffusion Experiments

## E. Other Current Topics in Diffusion Fundamentals

No.	Authors	Affiliation	Title
E1	<u>Subhasis Adhikari, Frank Cichos</u>	University of Leipzig	Probe Size Dependent Rotational Dynamics in Polymers by Single Molecule Spectroscopy
E2	<u>Ayan Chakrabarty, Feng Wang, Jonathan Selinger and Qi-Huo Wei</u>	Kent State University	Fabrication and Brownian Diffusion of Boomerang Colloidal Particles
E3	<u>S.Farshid Chini, Alidad Amirfazli</u>	University of Alberta	A Diffusive Model for Evaporation of Spherical Water Drops at Room Temperature and Standard Pressure
E4	<u>Mária Šoltésová, Ladislav Benda, Jiří Czernek, Jan Lang</u>	Charles University in Prague	Estimation of the Size of Alcohol Clusters through PFG NMR Diffusion Measurement

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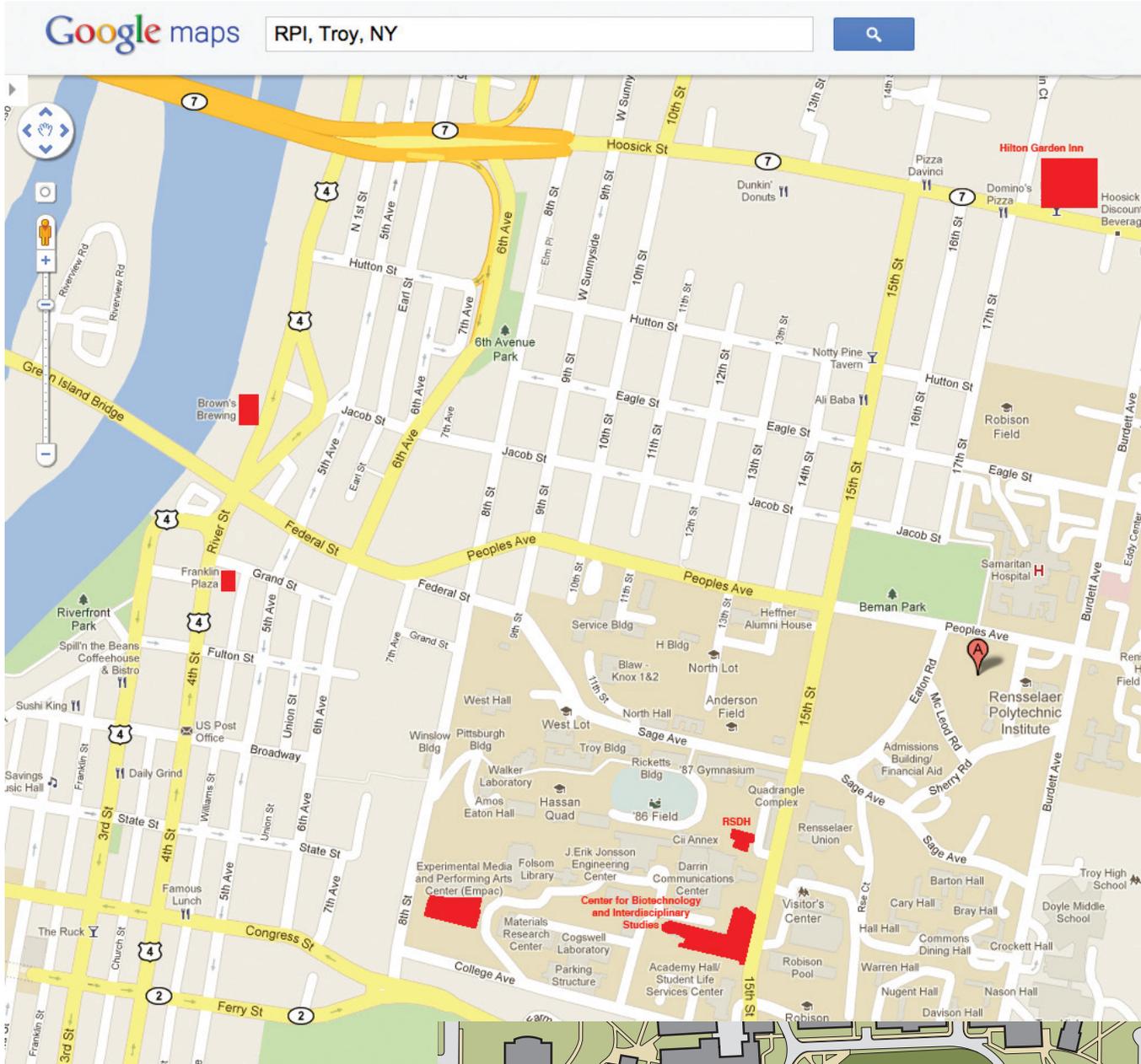
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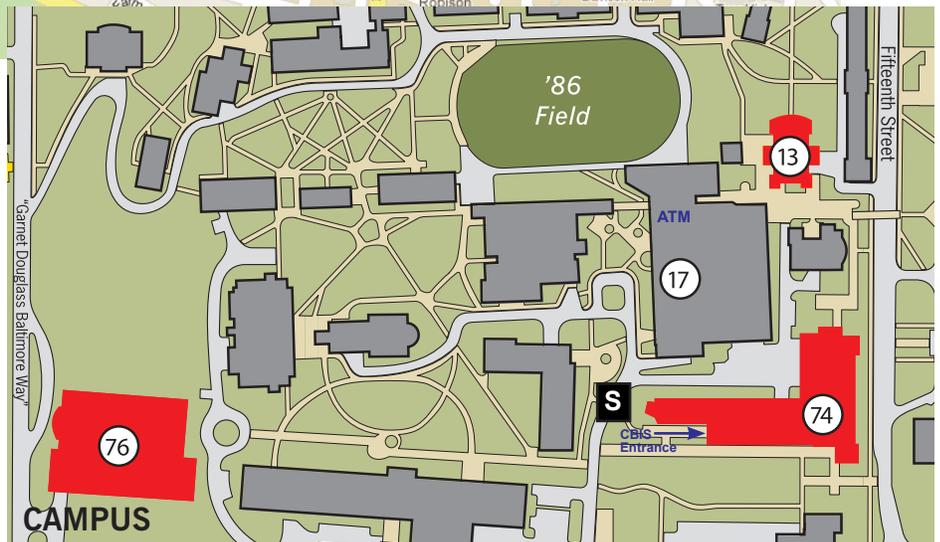
# Conference Locations

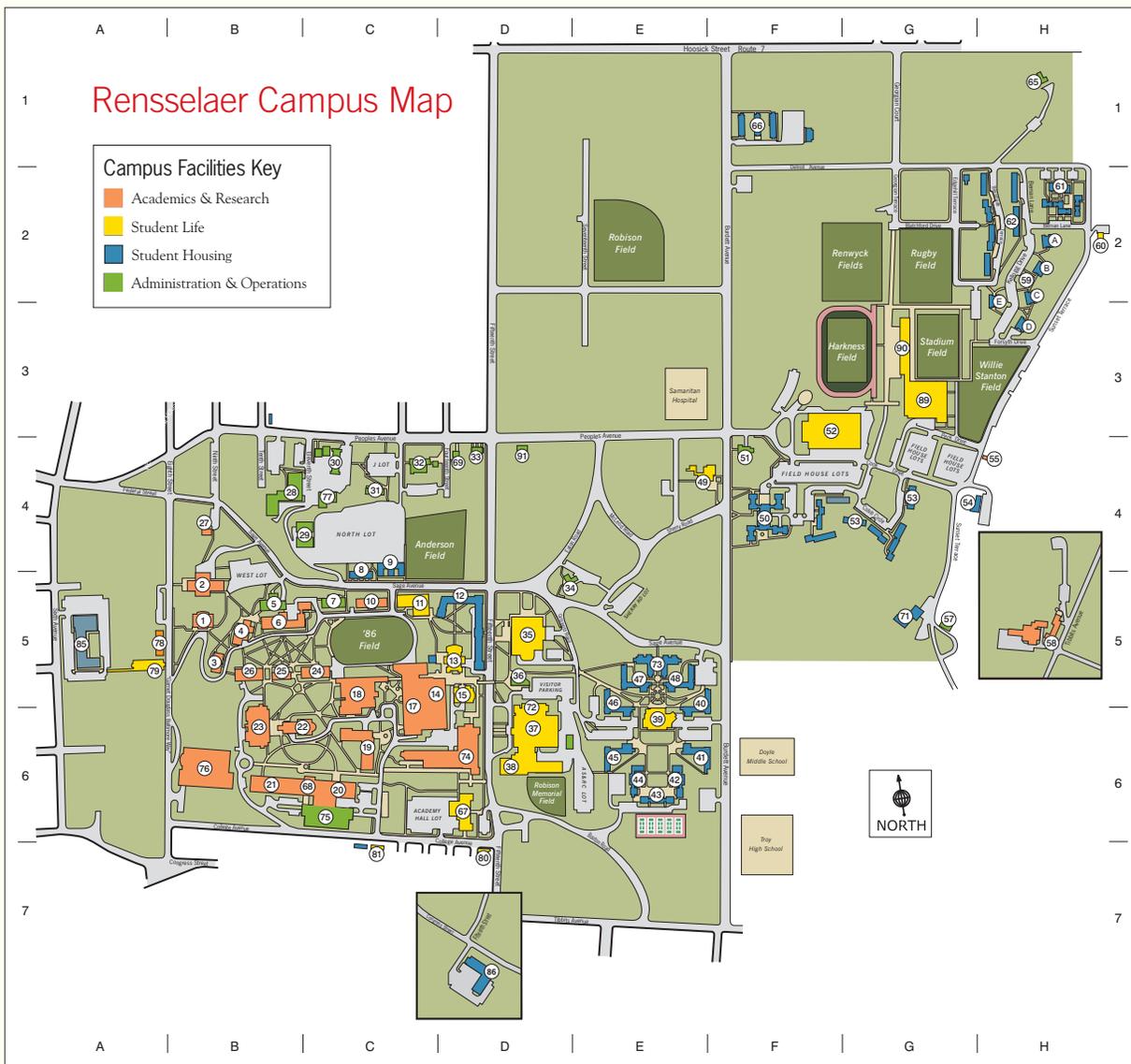


## Important Campus Locations:

- 74 - Center for Biotechnology and Interdisciplinary Studies (CBIS)
- 13 - Russell Sage Dining Hall
- 76 - Curtis R. Priem Experimental Media and Performing Arts Center (EMPAC)
- 17 - Darrin Communications Center — ATM location

**S** Hotel Shuttle Drop Off/Pick Up





#	Building Name	Map Location	#	Building Name	Map Location	#	Building Name	Map Location
67	Academy Hall (Financial Aid, Student Life Services Center, Health Center)	6D	68	Empire State Hall	6C	60	Radio Club W2SZ	2H
34	Admissions	5E	18	Engineering Center, J. Erik Jonsson	5C	53	Rensselaer Apartment Housing Project RAHP A Site (Single Students)	4G
32	Alumni House (Heffner)	4C	76	Experimental Media & Performing Arts Center (EMPAC)	6B	62	Rensselaer Apartment Housing Project RAHP B Site (Married Students)	2H
37	Alumni Sports & Recreation Center	6D	52	Field House, Houston	3F	35	Rensselaer Union	5D
26	Amos Eaton Hall	5B	23	Folsom Library	6B	10	Ricketts Building	5C
73	Barton Hall	5E	91	Graduate Education, 1516 Peoples Avenue	4D	38	Robison Swimming Pool	6D
69	Beman Park Firehouse	4D	24	Greene Building	5C	81	RPI Ambulance	7C
29	Blaw-Knox 1 & 2	4C	57	Greenhouses and Grounds Barn	5G	13	Russell Sage Dining Hall	5D
85	Blitman Residence Commons	5A	11	'87 Gymnasium	5C	6	Russell Sage Laboratory	5B
15	Boiler House, Sage Avenue	5B	31	H Building	4C	19	Science Center, Jonsson-Rowland (Hirsch Observatory)	6C
77	Boiler House, 11th Street	4C	46	Hall Hall	6E	55	Seismograph Laboratory	4H
48	Bray Hall	5E	30	J Building	4C	28	Service Building	4B
61	Bryckwyck	2H	80	Java ++ Cafe, 1527 Fifteenth Street	7D	43	Sharp Hall	6E
51	2144 Burdett Avenue	4F	25	Lally Hall	5B	59	Stacwyck Apartments	2H
50	Burdett Avenue Residence Hall	4F	58	LINAC Facility (Gaertner Laboratory)	5H	59A	Rousseau Apartments	2H
3	Carnegie Building	5B	79	Louis Rubin Memorial Approach	5A	59B	Williams Apartments	2H
47	Cary Hall	5E	21	Materials Research Center (MRC)	6B	59C	Wiltsie Apartments	2H
74	Center for Biotechnology and Interdisciplinary Studies (CBIS)	6D	72	Mueller Center	6D	59D	McGiffert Apartments	2H
14	Center for Industrial Innovation, Low (CII)	5D	41	Nason Hall	6E	59E	Thompson Apartments	2H
49	Chapel and Cultural Center	4E	27	41 Ninth Street	4B	71	133 Sunset Terrace	5G
20	Cogswell Laboratory	6C	8	North Hall	5C	54	200 Sunset Terrace	4H
66	Colonie Apartments	1F	44	Nugent Hall	6E	7	Troy Building	5C
39	Commons Dining Hall	6E	75	Parking Garage (Faculty/Staff)	6C	22	Voorhees Computing Center (VCC)	6C
40	Crockett Hall	5E	65	Patron Manor	1H	4	Walker Laboratory	5B
17	Darrin Communications Center (DCC)	6C	33	2021 Peoples Avenue	4D	45	Warren Hall	6E
42	Davison Hall	6E	1	Pittsburgh Building	5B	2	West Hall	5B
9	E Complex	5C	15	Playhouse	5D	78	Winslow Building	5A
89	East Campus Athletic Village Arena (ECAV)	3G	86	Polytechnic Residence Commons	7D			
90	East Campus Athletic Village Stadium	3G	36	Public Safety	5D			
			12	Quadrangle Complex	5D			

## **About Rensselaer Polytechnic Institute**

Rensselaer Polytechnic Institute is the nation's oldest technological university. The university offers degrees from five schools: Engineering; Science; Architecture; Humanities, Arts, and Social Sciences; and the Lally School of Management and Technology; as well as an interdisciplinary degree in Information Technology and Web Science.

Institute programs serve undergraduates, graduate students, and working professionals around the world. Students are encouraged to work in interdisciplinary programs that allow them to combine scholarly work from several departments or schools. The university provides rigorous, engaging, interactive learning environments and campus-wide opportunities for leadership, collaboration, and creativity at its campuses in Troy, N.Y., and in Hartford, Conn., as well as at its Southeastern Connecticut regional site and at the Center for Architecture Science and Ecology in New York City.

During the course of almost two centuries, Rensselaer has built a reputation for providing an undergraduate education of undisputed intellectual rigor based on educational innovation in the laboratory, classroom, and studio. In more recent years, driven by talented, dedicated, and forward-thinking faculty, Rensselaer has expanded dramatically its research enterprise by leveraging existing strengths and focusing on five signature research areas: biotechnology and the life sciences; computational science and engineering; experimental media and the arts; energy and the environment; and nanotechnology and advanced materials.

The Institute also has been a leader in the transfer of technology from the laboratory to the marketplace so that new discoveries and inventions benefit human life, protect the environment, and strengthen economic development.



The 220,000-square-foot Curtis R. Priem Experimental Media and Performing Arts Center (EMPAC) is a platform for the largely unexplored territory where art, science, and technology come together in ways that empower the creation of entirely new work that cannot be done anywhere else. Its linkage to the Center for Biotechnology and Interdisciplinary Studies and to the Computational Center for Nanotechnology Innovations is propelling Rensselaer to the scientific, engineering, and artistic frontiers of the 21st century.

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