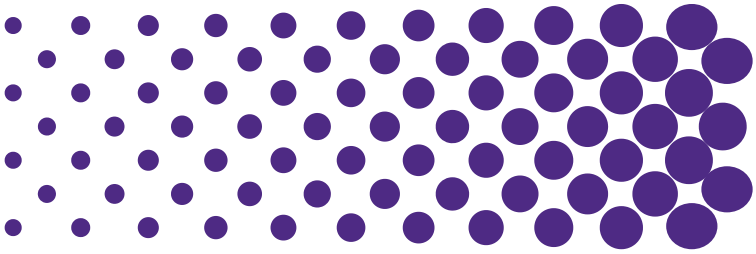
DIFFUSION FUNDAMENTALS XI



Diffusion Fundamentals XI

Spreading in Nature, Technology and Society

Louis Room, Norris University Center
1999 Campus Drive
Northwestern University
Evanston, IL 60208

Conference Organizers:
Randy Snurr Danny Abrams Todd Gingrich
Matthew Grayson Niall Mangan

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Spreading in Nature, Technology and Society
Diffusion Fundamentals XI

Northwestern University
Norris University Center, Louis Room
1999 Campus Drive, Evanston, IL 60208

Day 1: Monday June 30th

8:15 **Breakfast and Registration**
9:00 **Welcome**

Session Chair Lars Heinke

9:15 **Keynote Lecture: Monica Olvera de la Cruz**, Northwestern University, "Dynamics of Simple and Complex Electrolytes in Confinement"
9:50 Discussion
10:00 **Break**
10:30 **Cristián Huepe**, Northwestern University, "Contagion Dynamics in Active Agents"
10:50 Discussion
11:00 **Sotiris Pratsinis**, ETH Zürich, "Diffusion of Tiny Nanoparticles (TNPs) in Gases"
11:20 Discussion
11:30 **Dhairya Vyas**, Northwestern University, "Diffusion in Granular Mixtures"
11:50 Discussion

12:00 **Lunch and (optional) Information Session about Research Opportunities through the Alexander von Humboldt Foundation**

Session Chair Matthew Grayson

1:15 **Keynote Lecture: Stefano Brandani**, University of Edinburgh, "The Ruthven Number: An Essential Quantity in Determining Diffusion Coefficients in Nanoporous Materials Using Uptake Experiments"
1:50 Discussion
2:00 **Poster Lightning Talks** (8 x 3 minutes per person) Posters 1-8
2:30 **Break**
3:00 **Michael Goepel**, Leipzig University, "Diffusion in Nanoporous Materials in the Focus of an IUPAC Initiative: On the Benefit of Microscopic Measurement"
3:20 Discussion
3:30 **Yu Wang**, ExxonMobil Technology and Engineering, "Identification of Mass Transfer Resistances with Pressure-Swing Frequency Response"
3:50 Discussion
4:00 **Poster Lightning Talks** (8 x 3 minutes per person) Posters 9-16
4:30 **Poster Session 1** (odd numbered posters)
5:15 **Poster Session 2** (even numbered posters)
6:00 **End**

Day 2: Tuesday July 1st

8:30 **Breakfast**

Session Chair Danny Abrams

9:00 **Keynote Lecture: Mary Silber**, University of Chicago, "Semi-arid self-organizing vegetation patterns"
9:35 Discussion
9:45 **Duncan Burns**, Northwestern University, "Competition of Diffusion Modes at the Nanoscale: Dewetting and Sublimation"
10:05 Discussion
10:15 **Break**
10:45 **Matthew Grayson**, Northwestern University, "The Generalized Heavy-Tail Function: Fitting Slower-than-Exponential Relaxations in Complex Systems, Matter, & Molecules"
11:05 Discussion
11:15 **Edmund Seebauer**, University of Illinois at Urbana-Champaign, "Diffusive Isotopic Fractionation: Implications for Diffusion Modeling in Crystalline Solids"
11:35 Discussion
11:45 **János Tomán**, University of Debrecen, "Low-Temperature, Ultra-Giant Blistering of Atomic Layer Deposited Barrier Coatings on Polyethylene Films Caused by Additive Segregation"
12:05 Discussion

12:15 **Lunch**

Session Chair Todd Gingrich

1:30 **Keynote Lecture: Eric Vanden-Eijnden**, New York University, "Some Applications of Machine Learning in Active Matter"
2:05 Discussion
2:15 **John Zima**, Northwestern University, "Tensor Networks as an Alternative to Trajectory Sampling for Chemical Reaction Networks"
2:35 Discussion
2:45 **John Strahan**, Northwestern University, "Computing the Linear Response of Stationary Distributions Corresponding to Markov Processes with Rare Events"
3:05 Discussion
3:15 **Break**
3:45 **Rebecca Bivins**, Georgia Institute of Technology, "Comparing Solvent Diffusion in Carbon Molecular Sieve Membranes via Macroscopic Permeation and Pulsed-Field Gradient NMR"
4:05 Discussion
4:15 **William Price**, Western Sydney University, "Probing Reacting Systems with Diffusion NMR"
4:35 Discussion

Session Chair Randy Snurr

4:45 **Pre-Dinner Talk**: **Julio Ottino**, Northwestern University, "Determinism, Chaos, and Probability: Newton, Poincaré, and Maxwell"
5:45 **End**

7:00 **Conference Dinner**
Five & Dime Roof-top Deck
1026 Davis Street, Evanston, IL

Day 3: Wednesday July 2nd

8:30 **Breakfast**

Session Chair Hilal Daglar

9:00 **Keynote Lecture: Alberto Striolo**, University of Oklahoma, "Interrogating Transport Mechanisms in Crowded Narrow Pores Using Molecular Simulations"
9:35 Discussion
9:45 **Qinsi Xiong**, Northwestern University, "Modeling Ion Diffusion and Selective Transport in 2D Nanomembranes"
10:05 Discussion
10:15 **Break**
10:45 **Saifeldeen Abed Alrhman**, New York University, "Machine Learning Insights into H_2S Selective Diffusion in Metal–Organic Frameworks under Methane-Rich Conditions"
11:05 Discussion
11:15 **Faramarz Joodaki**, Northwestern University, "Computational Investigation of Chemical Warfare Agent Diffusion in Metal-Organic Frameworks in the Presence of Water"
11:35 Discussion
11:45 **Amber Mace**, Uppsala University, "Understanding Mobile Particles in Solid-State Materials: From the Perspective of Potential Energy Surfaces"
12:05 Discussion

12:15 **Lunch**

Session Chair Amber Mace

1:15 **Keynote Lecture: Charles Nicholson**, NYU Langone Health, "Diffusion Properties of Brain Interstitial Space"
1:50 Discussion
2:00 **Arindam Raj**, Northwestern University, "High Resolution Mapping of Diffusion Characteristics in General Microstructures"
2:20 Discussion
2:30 **Youri Ran**, University of Amsterdam, "RASPA3: A Monte Carlo Code for Computing Adsorption and Diffusion in Nanoporous Materials and Thermodynamic Properties of Fluids"
2:50 Discussion
3:00 **Break**
3:15 **Gergő Vecsei**, University of Debrecen, "The Effect of Stress on the Growth Kinetics of $ZnAl_2O_4$ in Cylindrical Nanotubes and Nanopillars"
3:35 Discussion
3:45 **Nicolas Chanut**, KU Leuven, "Diffusivity Measurements in Nanoporous Materials using a Temperature-Induced Desorption Approach"
4:05 Discussion
4:15 **Closing Remarks**
4:30 **Conference End**

Poster Presentations

1. **Tiong Wei Teh**, University of Stuttgart, “Multimodal study of self-diffusion nanoporous materials: experiment, molecular simulation and classical density functional theory”

2. **Michael Saxton**, UC Davis, “Lateral diffusion in an archipelago of biomembrane protuberances”

3. **Neha Tyagi**, Northwestern University, “Hydrodynamically-Enhanced Brownian motion in flowing polymer solutions”

4. **Barbara Sárközi**, University of Debrecen, “Interdiffusion and internal stress effects in closed geometry”

5. **Anagha Pushpa Balakrishnan**, Freie Universität Berlin, “Studying the Diffusion of Guest Molecule in the Nanopores of Metal-Organic Framework Thin Films”

6. **Emma Xiao**, State University of New York Downstate Health Sciences University, “The effect of dead-space microdomain entrance size and volume on brain extracellular space diffusion”

7. **Zoltán Erdélyi**, University of Debrecen, “Two-step reaction in oxides: nucleation and growth kinetics of $ZnAl_2O_4$ spinel in ZnO/Al_2O_3 bilayers”

8. **Zoltán Erdélyi**, University of Debrecen, “Reaction-diffusion in Co_2Si/Zn diffusion couple”

9. **Kaihang Shi**, University at Buffalo, “Fickian Diffusion Models for Interpreting Experimental Characterization of Mass Transfer in Nanoporous Materials”

10. **Cathyrn Murphy**, Northwestern University, “Tensor Networks for Estimating Reliability in Stochastic Low-Powered Circuits”

11. **Goda Pauryte**, University of Edinburgh, “Modelling the effects of bypass on flow systems working with mg-scale samples”

12. **Lucas Pham**, Northwestern University, “PEGylation of Carbon Black Yields Stable Colloidal Suspensions for Flow Battery Applications”

13. **Xi Wan**, Northwestern University, “Understanding ionic and electronic transport in composites with mixed ionic/electronic conducting layers coated on colloidal silica”

14. **Kayla Ghezzi**, Northwestern University, “Quantifying the Impact of Rotational Diffusion on Electron Transport in Dense Suspensions of Colloidal Rods”

15. **Geyao Gu**, Northwestern University, “It Takes Two to Make a Thing Go Right: Boosting Current in Coupled Motors”

16. **Hilal Daglar**, Koç University, “Investigating the Effects of Framework Flexibility on Water Adsorption in the Metal–Organic Framework NbOFFIVE-1-Ni via Molecular Modeling”