

## **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**

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 **Jörg Kärger**, 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 1<sup>st</sup>**

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 2<sup>nd</sup>**

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 **Saifelddeen Abed Alrhman**, New York University, “Machine Learning Insights into H<sub>2</sub>S 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<sub>2</sub>O<sub>4</sub> 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  $\text{ZnAl}_2\text{O}_4$  spinel in  $\text{ZnO}/\text{Al}_2\text{O}_3$  bilayers”
8. **Zoltán Erdélyi**, University of Debrecen, “Reaction-diffusion in  $\text{Co}_2\text{Si}/\text{Zn}$  diffusion couple”
9. **Kaihang Shi**, University at Buffalo, “Fickian Diffusion Models for Interpreting Experimental Characterization of Mass Transfer in Nanoporous Materials”
10. **Cathryn 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”