

## **Spreading in Nature, Technology and Society Diffusion Fundamentals XI**

*Northwestern University  
Norris Center, Louis Room*

### **Day 1: Monday June 30th**

- 8:30 **Breakfast and Registration**
- 9:00 **Welcome**
- 9:15 **Keynote Lecture:** TBD
- 10:00 **Break**
- 10:30 Cristián Huepe, “Contagion Dynamics in Active Agents”
- 11:00 Sotiris Pratsinis, “Diffusion of Tiny Nanoparticles (TNPs) in Gases”
- 11:30 Dhairya Vyas, “Diffusion in Granular Mixtures”
- 12:00 **Lunch**
- 1:15 **Keynote Lecture:** Stefano Brandani, “The Ruthven Number: An Essential Quantity in Determining Diffusion Coefficients in Nanoporous Materials Using Uptake Experiments”
- 2:00 **Poster Lightning Talks** (8 x 3 minutes per person) Posters 1-8
- 2:30 **Break**
- 3:00 Jörg Kärgler, “Diffusion in Nanoporous Materials in the Focus of an IUPAC Initiative: On the Benefit of Microscopic Measurement”
- 3:30 Yu Wang, “Identification of Mass Transfer Resistances with Pressure-Swing Frequency Response”
- 4:00 **Poster Lightning Talks** (7 x 3 minutes per person) Posters 9-15
- 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**
- 9:00 **Keynote Lecture:** TBD
- 9:45 Duncan Burns, “Competition of Diffusion Modes at the Nanoscale: Dewetting and Sublimation”
- 10:15 **Break**
- 10:45 Matthew Grayson, “The Generalized Heavy-Tail Function: Fitting Slower-than-Exponential Relaxations in Complex Systems, Matter, & Molecules”
- 11:15 Edmund Seebauer, “Diffusive Isotopic Fractionation: Implications for Diffusion Modeling in Crystalline Solids”
- 11:45 János Tomán, “Low-Temperature, Ultra-Giant Blistering of Atomic Layer Deposited Barrier Coatings on Polyethylene Films Caused by Additive Segregation”
- 12:15 **Lunch**

- 1:30 **Keynote Lecture:** Eric Vanden-Eijnden, “Some Applications of Machine Learning in Active Matter”
- 2:15 John Zima, “Tensor Networks as an Alternative to Trajectory Sampling for Chemical Reaction Networks”
- 2:45 John Strahan, “Computing the Linear Response of Stationary Distributions Corresponding to Markov Processes with Rare Events”
- 3:15 **Break**
- 3:45 Rebecca Bivins, “Comparing Solvent Diffusion in Carbon Molecular Sieve Membranes via Macroscopic Permeation and Pulsed-Field Gradient NMR”
- 4:15 William Price, “Probing Reacting Systems with Diffusion NMR”
- 4:45 **Pre-Dinner Talk:** Julio Ottino, “Determinism, Chaos, and Probability: Newton, Poincaré, and Maxwell”
- 5:45 **End**
- 7:00 **Conference Dinner**

**Day 3: Wednesday July 2<sup>nd</sup>**

- 8:30 **Breakfast**
- 9:00 **Keynote Lecture:** Alberto Striolo, “Interrogating Transport Mechanisms in Crowded Narrow Pores Using Molecular Simulations”
- 9:45 Qinsi Xiong, “Modeling Ion Diffusion and Selective Transport in 2D Nanomembranes”
- 10:15 **Break**
- 10:45 Saifelddeen Abed Alrhmman, “Machine Learning Insights into H<sub>2</sub>S Selective Diffusion in Metal-Organic Frameworks under Methane-Rich Conditions”
- 11:15 Faramarz Joodaki, “Computational Investigation of Chemical Warfare Agent Diffusion in Metal-Organic Frameworks in the Presence of Water”
- 11:45 Amber Mace, “Understanding Mobile Particles in Solid-State Materials: From the Perspective of Potential Energy Surfaces”
- 12:15 **Lunch**
- 1:15 **Keynote Lecture:** Charles Nicholson, “Diffusion Properties of Brain Interstitial Space”
- 2:00 Arindam Raj, “High Resolution Mapping of Diffusion Characteristics in General Microstructures”
- 2:30 Youri Ran, “RASPA3: A Monte Carlo Code for Computing Adsorption and Diffusion in Nanoporous Materials and Thermodynamic Properties of Fluids”
- 3:00 **Break**
- 3:15 Gergő Vecsei, “The Effect of Stress on the Growth Kinetics of ZnAl<sub>2</sub>O<sub>4</sub> in Cylindrical Nanotubes and Nanopillars”
- 3:45 Nicolas Chanut, “Diffusivity Measurements in Nanoporous Materials using a Temperature-Induced Desorption Approach”
- 4:15 **Closing Remarks**
- 4:30 **Conference End**

## Poster Presentations

1. Tiong Wei Teh, "Multimodal study of self-diffusion nanoporous materials: experiment, molecular simulation and classical density functional theory"
2. Michael Saxton, "Lateral diffusion in an archipelago of biomembrane protuberances"
3. Neha Tyagi, "Hydrodynamically-Enhanced Brownian motion in flowing polymer solutions"
4. Barbara Sárközi, "Interdiffusion and internal stress effects in closed geometry"
5. Anagha Pushpa Balakrishnan, "Studying the Diffusion of Guest Molecule in the Nanopores of Metal-Organic Framework Thin Films"
6. Emma Xiao, "The effect of dead-space microdomain entrance size and volume on brain extracellular space diffusion"
7. Zoltán Erdélyi, "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, "Reaction-diffusion in  $\text{Co}_2\text{Si}/\text{Zn}$  diffusion couple"
9. Kaihang Shi, "Fickian Diffusion Models for Interpreting Experimental Characterization of Mass Transfer in Nanoporous Materials"
10. Cathryn Murphy, "Tensor Networks for Estimating Reliability in Stochastic Low-Powered Circuits"
11. Goda Pauryte, "Modelling the effects of bypass on flow systems working with mg-scale samples"
12. Lucas Pham, "PEGylation of Carbon Black Yields Stable Colloidal Suspensions for Flow Battery Applications"
13. Xi Wan, "Understanding ionic and electronic transport in composites with mixed ionic/electronic conducting layers coated on colloidal silica"
14. Kayla Ghezzi, "Quantifying the Impact of Rotational Diffusion on Electron Transport in Dense Suspensions of Colloidal Rods"
15. Geyao Gu, "It Takes Two to Make a Thing Go Right: Boosting Current in Coupled Motors"