

NANOFLUIDICS 2026

Lake Tahoe



February 8-12th 2026
Granlibakken-at-Tahoe
Tahoe City, California USA

Organizers

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Welcome Note

Welcome to Nanofluidics 2026, held in Lake Tahoe, California, at the Granlibakken Tahoe Resort and Conference Center.

Nanofluidics 2026 is conceived as a focused, discussion-driven workshop that brings together researchers working at the forefront of nanofluidics, ion transport, membrane science, and related nanoscale phenomena. Beyond the presentation of new results, the conference aims to foster a strong sense of community through open scientific exchange and close interaction among invited speakers, oral contributors, poster presenters, and participants from diverse disciplinary backgrounds.

In contrast to large-scale conferences, Nanofluidics 2026 emphasizes depth over breadth. The program features carefully selected oral presentations, extended discussion periods, and dedicated poster sessions, creating an environment that encourages open dialogue, constructive feedback, and the sharing of ideas at all stages of development. Informal interactions are an integral part of the meeting, supporting meaningful scientific conversations and the formation of lasting professional connections.

The setting at Granlibakken Tahoe provides a retreat-style environment that naturally encourages interaction beyond the lecture room. By combining a focused scientific program with ample opportunities for informal discussion, the conference is designed to strengthen connections within the nanofluidics community and to support both established researchers and early-career scientists, including students and postdoctoral scholars.

We are grateful to all speakers and contributors for sharing their work, and to the poster presenters for enriching the scientific discussions. We also thank our sponsors for their generous support, which makes this meeting possible.

We hope that Nanofluidics 2026 offers a welcoming and inclusive forum for scientific exchange, inspires new collaborations, and contributes to the continued growth of the nanofluidics community.

We wish you a productive and enjoyable conference.

Enjoy the conference and the snow!

The Organizing Committee

Nanofluidics 2026

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Part I. Main Agenda

Day 1 – Sunday, Feb 08, 2026

10:10 am – Arrivals

06:00 pm – Welcome reception and dinner

Day 2 – Monday, Feb 09, 2026

07:00 am – Breakfast

08:00 am – Seth Darling

Membranes by Design: Engineered Phyllosilicate Laminates for Ion-Ion Separations

08:20 am – Cody Ritt

Leveraging Nanofluidics to Engineer Practical Separation Materials for Water and Energy Needs

08:35 am – Mainak Majumder

Selectivity via Transport Energy Barriers in Practical Graphene Oxide Membranes

08:50 am – Narayana Aluru

Solvent-Mediated Ionic Memory

09:10 am – Yoav Green

Goldman-Hodgkin-Katz Equation, Reverse Electrodialysis, and Everything in Between

09:25 am – Liangwei Zheng

Turning Failure into Function: New Applications of Nanoparticle-Blocked Nanopores

09:40 am – Coffee Break

10:10 am – Kumar Varoon Agrawal

Mechanistic-Insight based Fabrication and Scale-Up of Graphene Membrane Hosting Single Digit Pores

10:30 am – Mohit Saraswat

Mechanosensitive Ion Transport in Hexagonal Boron Nitride Nanopores

10:45 am – Chong Liu

Dialing the Energy Landscape in Ångström-Scale Confinement for Separation

11:05 am – Pengzhan Sun

Molecular and Ionic Sieving across 2D Angstromporous Membranes

11:20 am – Jerry W. Shan

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Comparing Transport in Carbon-Nanotube, Boron-Nitride-Nanotube and Heterostructured-CNT-BNNT Membranes

11:35 am – Free Afternoon

05:30 pm – Dinner

07:05 pm – Tuan Anh Pham

Quantum Effects in Nanofluidic Transport: From Electrons to Ions

07:25 pm – Peter Berg

A Multiscale Framework for the Analysis of Nanobubbles in Nanoconfined Domains

07:40 pm – Alessandro Siria

Synergistic Nanofluidics Between Soft and Hard Condensed Matter

08:00 pm – 10:00 pm – Posters & Happy Hour

Day 3 – Tuesday, Feb 10, 2026

07:00 am – Breakfast

08:00 am – Aleksandra Radenovic

Opening the Black Box: Operando Microscopy Transforms Nanofluidics

08:20 am – Jie Shen

Next-Gen 2D Membranes with Ordered, Atomically Precise Channels

08:35 am – Hyung Gyu Park

Angstrofluidics in 2D Molybdenum Disulfide Channels

08:50 am – Marija Drndić

Breakdown of Conductance Scaling in Atom-Scale Artificial Ion Channels

09:10 am – Gideon Segev

Experimental Demonstration of Ambipolar Ion Transport with Ratchet-Based Ion Pumps

09:25 am – Jobaer Abdullah

Chirality-Dependent Rare Earth Ion Transport and Separations in Carbon Nanotube Porins

09:40 am – Coffee Break

10:10 am – Ping Yu

Polyelectrolyte Brushes-Confined Nanofluidics

10:30 am – Marcelo Losada Hidalgo

Field Effects in Proton Transport through 2D Crystals

10:45 am – Rohit Karnik

Nanoporous Atomically Thin Membranes for Challenging Chemical Separations

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11:05 am – Joan M. Montes de Oca

Engineering Non-Equilibrium Electrostatics in Bipolar Nanopores

11:20 am – Piran R. Kidambi

Atomically Thin Proton Exchange Membranes: Synthesis, Processing, and Device Integration

11:35 am – Free Afternoon

05:30 pm – Dinner

07:05 pm – Viatcheslav Freger

Ion Permeability vs. Thickness: Fundamental Limitations and Curious Opportunities for Ultrathin Films

07:25 pm – Yahui Xue

Mimicking Biological Ion Channels Using Voltage-Gated Graphene Nanochannels

07:40 pm – Aleksei Aksimentiev

Rotating Helices in Nanoscale Pores

08:00 pm – 10:00 pm – Posters & Happy Hour

Day 4 – Wednesday, Feb 11, 2026

07:00 am – Breakfast

08:00 am – Slaven Garaj

Frictionless Flow of Surface Ions in 2D nanopores

08:20 am – Zhongwu Li

Neuromorphic Ionic Computing in Droplet-Based Biomimetic Synapses

08:35 am – Amir Haji-Akbari

Few and Far in Between: Probing the Structure-Selectivity Relationship in Membranes using Path Sampling Techniques

08:50 am – Nikita Kavokine

Nanofluidics beyond the Wall

09:10 am – Anna Drummond Young

Decoding Noise in Nanofluidic Systems: Adsorption vs Diffusion Signatures in Power Spectra

09:25 am – Takeru Okada

Effect of Flow Conditions on Electricity Generation at Interface Between Graphene and Flowing Water in Fluidic Channel

09:40 am – Coffee Break

10:10 am – Zuzanna Siwy

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Nanopores with Dynamic Pore Opening Diameter for the Design of Ionic Memory Systems

10:30 am – Andy W.C. Lau

Theory of Friction for One-Dimensional Water Structures Moving through A Sub-Nanometer Carbon Nanotube

10:45 am – Radha Boya

Water and Ions in Angstrom-Scale Channels Made from 2D Materials

11:05 am – Yuewen Jia

Mixed Ion Transport in Confined Nanochannels of Microporous Polymer Membranes

11:20 am – Aida Fica

Tissue-like Jammed Emulsions: An Emerging Biomimetic Architecture Towards Defect-free Ion Channel-based Membranes

11:35 am – Free Afternoon

05:45 pm – Mihail Barboiu

Pillararene Water Channels - Structural Determinants for Enhanced Filtration Performances in Bilayer and Polymeric Membranes

06:05 pm – Armin Götzhäuser

Passage of Gases and Vapors through Nanoporous Two-Dimensional Carbon Nanomembranes (CNMs)

06:20 pm – Guang Chen

Non-Monotonic Salt Dependence of Electro-Osmotic Flow in pH-Regulated Nanochannels

06:35 pm – Closing remarks

07:00 pm – Conference banquet dinner and awards

Day 5 – Thursday, Feb 12, 2026

07:00 am – Breakfast

12:00 pm – Departures

Part II. Poster Agenda

Day 2 – Monday, Feb 09, 2026

08: 00 pm – 10:00 pm – Posters & Happy Hour

Day 3 – Tuesday, Feb 10, 2026

08: 00 pm – 10:00 pm – Posters & Happy Hour

Jacob Bair

(Poster 1) Interpore Coupling Effects on the Spreading Resistance of A Nanopore Pair

Pia Bhatia

(Poster 2) Coupled Nanopore Devices Towards Advanced DNA and Protein Sequencing

Anthony Dougman Cho

(Poster 3) High-Dimension Ionic Memory in Oscillating Ion Current Signals

Claudia E. P. Dewi

(Poster 4) Enhancing Conductance of Two-Nanopore Arrays using Dual-Barrel Nanopipettes with Individual-Pore Electrochemical Tunability

Jiachen Feng

(Poster 5) Engineering Synthetic Macrocycles for Selective Rare Earth Elements Separation

Sanjay S. Garimella

(Poster 6) Formulation and Validation of A Nanoconfined Equation of State using Thermally Driven Isobars Within Single Digit Nanopores

Peter Gispert

(Poster 7) Electronic Friction in Single-Digit Carbon Nanotubes and Quantum Osmosis

Alon Herman

(Poster 8) Ratcheting Up Selectivity: A New Paradigm in Ion Separation

Eli Hoenig

(Poster 9) Control of Li Transport and Heterogeneous Charge Transfer Using Dual Electrolyte Gating

Sabine Hong

(Poster 10) Solid-State Nanopore-Informed Technique for Statistical Modeling of Single-Molecule Protein Folding

Rachael N. Keneipp

(Poster 11) Demonstration of A New Ionic Conductance Regime in Extremely Confined Nanopores

Omar Khalifa

(Poster 12) Ion Transport in Nanoporous Membranes: The Effect of Pore Length and Chemistry

Jingyi Li

(Poster 13) Iontronic Synaptic Behaviors of Nanopipettes

Xinxin Liu

(Poster 14) Particle-gated, Ionically Driven Nanocantilever with Memristive Hysteresis in Liquid

Hao Lu

(Poster 15) Electronic Correlations in 2D Materials Induced by Interfacial Water

Celia Morral

(Poster 16) Reversible Nanopore sealing via in situ Iron Oxide Synthesis

Killian Rigaux

(Poster 17) Measuring Nanoscale Flows with Quantum Sensing

Marco Rolandi

(Poster 18) Interfacing Natural and Artificial Membrane Channels with Ion Selective Bioelectronics

Mohit Saraswat

(Poster 19) Mechanosensitive Ion Transport in Hexagonal Boron Nitride Nanopores

Matthew Schiel

(Poster 20) Stacked 2D Materials for Temporal Gating of Ion Transport through Nanopores with both DC and AC Gate Voltages

Ayelet Ben-Kish Sharvit

(Poster 21) Towards a Unified Understanding of the Electrical Response of Bipolar Nanofluidic Systems

Savannah Silva

(Poster 22) Nanopores with Dynamic Pore Opening Diameter

Jay Prakash Singh

(Poster 23) Ion Pairing in Osmotically-Stressed Environment: Disentangling the Effects of Ion-Ion and Ion-Water Interactions

Shiwei Tang

(Poster 24) Memory in Conical Nanopores Regulated by Electrolyte Composition and Pore Size

Jarrett S. Turner

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(Poster 25) Predicting Adsorption Length Scales in Nanoconfined Fluids: Applications to Generalized van der Waals Confined Equations of State

Camille Violet

(Poster 26) Ion Transport through Single-crystal MOF Membranes

Zhen Yao

(Poster 27) Scalable and Tunable Carbon Nanomembranes for Selective Molecular Transport

Sangeeta Yadav

(Poster 28) Two-dimensional Clay Channels for Tunable Nanofluidic Memristor

Kalluvadi Veetil Saurav

(Poster 29) Direct Imaging Reveals Electromechanical Blistering-based Ionic Memory in Two-Dimensional Nanochannels

Part III. Oral Abstracts

Membranes by Design: Engineered Phyllosilicate Laminates for Ion-Ion Separations

Authors: Yining Liu, Mina Kim, Austin Booth, Shao Wei Tsai, Zijing Xia, Bratin Sengupta, George Schatz, Ilya Shkrob, Noah Paulson, Jeffrey Elam, Seth B. Darling

Affiliation: Argonne National Laboratory, USA

Abstract: Layered phyllosilicates offer a uniquely tunable inorganic platform for nanofluidic membranes capable of precise ion manipulation under extreme spatial confinement. By leveraging liquid-phase exfoliation, controlled crosslinking, and functionalization, we construct laminar membranes with angstrom-level control over interlayer spacing, surface charge, and channel topology. These engineered galleries function as well-defined 1D–2D nanofluidic conduits whose transport properties diverge markedly from those of conventional polymeric membranes, enabling systematic exploration of valence-, size-, and charge-based selectivity. We demonstrate how cation doping and crosslinker architecture modulate nanofluidic transport regimes, switching channel polarity, narrowing pore dimensions, and enhancing both monovalent/multivalent discrimination and fine size cutoffs. Extending these concepts, we establish a high-throughput autonomous platform capable of characterizing large libraries of mineral-based nanofluidic membranes, accelerating materials discovery toward energy-critical separations and resource recovery. This work positions naturally abundant clays as a customizable and scalable foundation for next-generation nanofluidic systems with application-relevant selectivity and robustness.

Leveraging Nanofluidics to Engineer Practical Separation Materials for Water and Energy Needs

Authors: Cody Ritt

Affiliation: University of Colorado, Boulder

Abstract: Achieving global water and energy security necessitates the use of unconventional sources (e.g., industrial brine) to augment our supply of both resources. This requires fit-for-purpose separations tailored to the product(s) of interest. Membrane-based separations are well-suited for addressing these challenges due to their energy efficiency and modularity; however, existing nanoporous membrane materials lack the molecular selectivity needed for these complex, new-age water resources. Hence, this research aims to leverage nanofluidic principles to elucidate the synthesis–structure–performance relationships needed for increased selectivity in practical nanoporous membranes and to provide perspective on material solutions. This work identifies critical design bottlenecks for engineering molecular selectivity into nanoporous membranes formed by either flexible polymers or rigid two-dimensional (2D) crystals such as graphene. Contextualizing the findings from both nanoporous systems, I introduce 2D polyaramids—which marry the rigid structure of 2D crystal analogues with the synthetic processability of traditional polymers—as ideal candidates for the next generation of nanofluidic separation materials.

Selectivity via Transport Energy Barriers in Practical Graphene Oxide Membranes

Authors: Mainak Majumder

Affiliation: Monash University

Abstract: Membrane-based separation technologies have many advantages over traditional separation methods such as adsorption, and distillation in terms of energy- and cost-efficiency and modular deployment of technology. In practice, these advantages can be meaningfully harnessed only if advanced membranes with properties such as high permeance, tailorable selectivity [1-2], chlorine, pH and solvent resistance [3-4], low-fouling characteristics [1], long-term stability under operational conditions [5,6] alongside green and sustainable manufacturability [6] are demonstrated. In the last 8-10 years, our research group has taken rapid strides to realize these properties in membranes made from graphene-oxide, including scaled-up manufacturing in roll-to-roll approaches.

Recently, our efforts have been focused on tailoring the interpore energy barriers in the graphene oxide nanochannels to impart selectivity which are non-classical, determined primarily by interactions from confined molecules. With this philosophy we have been able to separate short-chain per- and polyfluoroalkyl substances and concentrate them with efficiencies higher than what commercial membranes are capable of [7].

In this talk, I will summarize this journey reflecting on our work including pilot scale trials of spiral wound membrane modules conducted in close collaboration with industry partners and water utility companies.

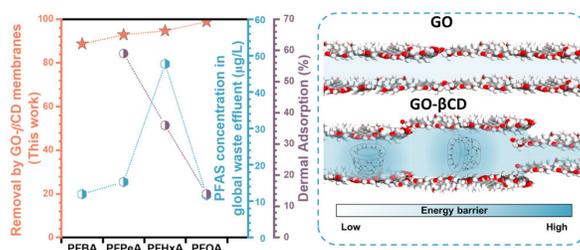


Fig. 1. Energetic transport barriers by incorporating Cyclodextrin cages inside Graphene Oxide nanochannels

References:

- [1] Akbari et al., *Nat Commun* 7, 10891 (2016),
- [2] Sheath et al., *Phil. Trans. R. Soc. A* 374: 20150028,
- [3] Akbari et al., *ACS Appl. Mater. Interfaces* 2018, 10, 2, 2067–2074,
- [4] Meragawi et al., *ACS Appl. Bio Mater.* 2020, 3, 1, 584–592,
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- [7] Mahofa et al., *ACS Nano.*, 2025, 19, 14742–14755

Solvent-Mediated Ionic Memory

Authors: Narayana R Aluru

Affiliation: Oden Institute for Computational Engineering and Sciences, Department of Mechanical Engineering, The University of Texas at Austin, Austin, TX

Abstract: Nanofluidic memristors have received significant attention over the last few years. History dependent ionic conduction has been realized using various mechanisms including electrowetting, concentration polarization, ion adsorption/desorption, the Wien effect, electrostriction, etc. In this talk, we introduce a solvent structure, and dynamics mediated memory in an Å-scale channel and pore connecting two electrolyte reservoirs. Using molecular dynamics simulations, we find pronounced I - E (current-electric field) hysteresis in ion conduction across various solvents and their mixtures. The hysteresis originates from the coupled evolution of in-channel ion concentration and hydrogen bond network order, i.e., elevated ion concentrations in the channel at high electric fields disrupt solvent ordering and enhance ion mobility by lowering solvent drag. In addition to ionic memory, we also introduce negative differential resistance (NDR) and reveal the role of the solvent.

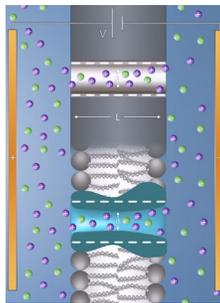
Goldman-Hodgkin-Katz Equation, Reverse Electrodialysis, and Everything in Between

Authors: Yoav Green

Affiliation: Department of Mechanical Engineering, Ben-Gurion University of the Negev, Israel

Abstract: In the past 80 years, the Goldman-Hodgkin-Katz (GHK) equation has been the gold-standard framework for interpreting countless biological/physiological experiments that involve ion transport in nanopores, nanochannels, and ion-channels subjected to a combined ionic concentration and electric potential gradients. In parallel to GHK, the reverse electrodialysis (RED) community, which utilizes the same framework to model energy harvesting, has developed its own mathematical model, which is non-commutative with GHK, and makes substantially different predictions.

I will review the mathematical foundations of both the GHK and RED models. I will show that GHK's infamous assumption of a constant electric field is incorrect, which leads to substantial errors, including the inability of this model to satisfy electroneutrality. I will then show how RED's approach of requiring electroneutrality leads to a non-constant electric field and entirely different predictions. Another advantage of the new RED model [1,2] is that, in contrast to GHK, which assumes that the surface charge density is negligible, in the new model, the effects of the surface charge density need not be negligible. Importantly, all of our newly derived results show remarkable correspondence to non-approximated numerical simulations. Our recent works [1,2] provide a brand-new framework for interpreting ion transport experiments in any charge-selective system.



References:

- [1] Y. Green, Goldman-Hodgkin-Katz Equation, Reverse Electrodialysis, and Everything in Between, *Phys. Rev. E* 111, 064408 (2025).
- [2] Y. Green, Universal Model for Ion Transport: Bridging The Goldman-Hodgkin-Katz Paradigm with Reverse Electrodialysis, *Phys. Rev. Lett.* 134, 228401 (2025).

Turning Failure into Function: New Applications of Nanoparticle-Blocked Nanopores

Authors: Liangwei Zheng, Jiayi Xu, Yiding Zhong, Bernie Xu, Chuanhua Duan

Affiliation: Department of Mechanical Engineering, Boston University

Abstract: Clogged nanopores have traditionally been viewed as a failure in nanopore research over the past three decades. Recent studies, however, reveal that nanoparticle-blocked nanopores can generate novel transport phenomena and enable new applications, suggesting a promising direction in nanofluidics and nanopore research. Here we highlight two applications. First, we demonstrate a blockage-based nanopore array assay for rapid, ultrasensitive nanoparticle detection. Fluorescent nanoparticles are driven through sub-nanoparticle-sized pores under hydraulic pressure, and optical microscopy monitors progressive blockage. Our results show that the initial blockage rate scales linearly with concentration, enabling detection down to 0.5 aM (≈ 300 particles/mL) within 5 minutes—five-order-of-magnitude more sensitive than prior nanopore methods. Fluorescent nanoparticles also act as probes to detect unlabeled nanoparticles and contaminants at similarly low concentrations, offering a versatile platform for biomedical, environmental, and industrial sensing. Second, we introduce a nanofluidic memristor formed by nanoparticle-blocked pores that create ultrasmall, asymmetric ionic confinement. This structure induces strong ion polarization under electric fields, producing memristive behavior with pinched I–V hysteresis. The system also exhibits clear frequency and concentration dependence, and demonstrates basic neuromorphic functions such as short-term potentiation and depression. These findings challenge the conventional view of clogged nanopores and open new avenues for nanoscale sensing and neuromorphic device development.

Mechanistic-Insight based Fabrication and Scale-Up of Graphene Membrane Hosting Single Digit Pores

Authors: Kumar Varoon Agrawal

Affiliation: Laboratory of Advanced Separations, École Polytechnique Fédérale de Lausanne (EPFL), Sion, Switzerland

Abstract: Porous two-dimensional selective films where pores act as zero-dimensional aperture are highly attractive for rapid permeation of molecules where one can tune molecular transport, and therefore, molecular selectivity and flux by tuning pore size and pore edge functional groups. Porous single-layer graphene film is emerging as a highly attractive candidate to achieve ultrahigh flux given that it is just one atom thick, and that the scale-up of large area graphene by chemical vapor deposition is already successful. However, pore formation in graphene remains stochastic with trial-and-error approaches used for pore formation.

Controlled oxidative pore formation in graphene, e.g., using ozone, is highly attractive because one can decouple the events that leads to pore nucleation and growth. This allows one to control pore size by systematic oxidant exposure. A series of surface events takes place during oxidation, involving chemisorption of epoxies, their surprisingly organized clustering, and strain-led gasification ultimately yielding a Å-scale pore. Ordered clustering of epoxies takes place from energy-minimizing cooperative assembly forming cyclic trimers followed by linear chains of trimers, chain-chain coalescence, and finally an ordered honeycomb superstructure. The degree of order in these clusters is highly surprising mainly because oxidized graphene domains were once thought to be amorphous. Luckily, it is opening new avenues to control the pore size, e.g., by a controlled gasification of the cluster. Our recent molecular dynamics simulations based study reveal that semiquinone group, incorporated at the pore edge by gasification, are highly dynamic, allowing surprising selective separation, even from large pores which were initially thought to be nonselective. The pore environment becomes highly dynamic with functional groups allowing CO₂ to pass through seemingly impermeable pores.

The knowledge of edge functional group surrounding graphene pore, previously inaccessible by the microscopy studies, allows one to also carry out controlled gasification and functionalization. For example, pyridinic N at the pore remarkably improve the CO₂/N₂ separation performance of the pore. Next, large-area membranes using simple method is demonstrated with unprecedented reproducibility, thanks to the simplified chemistry of forming pores, and out-of-box approach of using gas-permeable mechanical-reinforcing film on graphene. Field trial of these membranes for point-source carbon capture using industrial flue gas shows highly promising results.

References:

- [1] Villalobos, L. F.; Babu, D. J.; Hsu, K.; Van Goethem, C.; Agrawal, K. V., Gas Separation Membranes with Atom-Thick Nanopores: The Potential of Nanoporous Single-Layer Graphene. *Accounts Mater. Res.* 3, 1073–1087, 2022.
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Mechanosensitive Ion Transport in Hexagonal Boron Nitride Nanopores

Authors: Mohit Saraswat^{1,2}, Dana O. Byrne³, Yechan Noh^{3,4}, Alex T. Hall⁵, Sanjin Marion⁶, Julia Chung¹, Aleksandra Radenovic⁷, Alex Smolyanitsk⁴, John Cummings⁵, Frances Allen³, Aleksandr Noy^{1,2}

Affiliation: ¹Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, CA 94550 USA; ²School of Natural Sciences, University of California Merced, Merced, CA 95343 USA; ³Department of Chemistry, University of California Berkeley, Berkeley, CA, USA; ⁴National Institute of Standards and Technology, Boulder, CO USA; ⁵Department of Materials Science and Engineering, University of Maryland, College Park, MD, 20742 USA; ⁶Interuniversity Microelectronics Centre (IMEC), Belgium; ⁷École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Abstract: Achieving dynamic control over ion transport at the atomic scale is a major requirement for the development of next generation nanofluidic devices. Applied mechanical strain represents an almost completely unexplored control parameter. We have studied the impact of small lateral strains applied to nanopores in single-layer hexagonal boron nitride (hBN) on ion current through those nanopores. Our experimental setup uses hydrostatic pressure applied to a porous hBN flake mounted on flexible membrane support to transmit lateral strain to the nanopore. Our findings indicate that modest 2% strains induce significant (up to 30%) and reversible changes in ionic conductance, and that these changes cannot be attributed to streaming current or geometric pore dilation. Our results provide direct experimental validation of recent theoretical predictions for mechanosensitivity of ion transport in hBN nanopores, establish a mechanistic framework for strain-tunable ion transport in 2D membranes, and open up new pathways to develop nanofluidic systems with tunable selectivity and performance for applications in filtration, sensing, and energy harvesting.

Keywords: Mechanosensitive transport, Nanofluidics, Single digit nanopores, hexagonal boron nitride, 2D materials

Dialing the Energy Landscape in Ångström-Scale Confinement for Separation

Authors: Chong Liu

Affiliation: University of Chicago, USA

Abstract: Fluids in nanometer-scale or Ångström-scale create a unique chemical environment that invokes water and ion behaviors markedly different from those observed in the bulk. Ångström-scale confinement provides a distinctive opportunity to study water and ion transport and separation, leveraging solvated ion sizes and solid-state migration energy barriers. In this talk, I will introduce our group's effort in creating materials platforms that can be utilized as solid ionic channels with Ångström-scale confinement. We reveal the importance of the structural features and responses of the channel materials in dialing the energy differences along the transport pathway for separation. Moreover, when the ion transport is associated with the valence change of the solid channel materials, the crystal symmetry and vacancy level become critical in governing the energy landscape.

Molecular and Ionic Sieving across 2D Angstromporous Membranes

Authors: Pengzhan Sun

Affiliation: Institute of Applied Physics and Materials Engineering, University of Macau, Macau SAR, China

Abstract: It is widely believed that, despite being one-atom thick, graphene and other 2D crystals is completely impermeable to all gases and liquids. In this talk, I will update our recent research¹⁻⁵ on the topic “Molecular and ionic sieving across 2D angstromporous membranes”.

Using monocrystalline container made from atomically flat graphite, which is tightly sealed with graphene, we have achieved measurements that put the permeation limit through 2D materials at 8–9 orders of magnitude lower than previously, such that we would discern (but did not observe) just a few helium atoms per hour crossing micrometer-size membranes. This detection limit is also valid for all other gases tested, except for hydrogen. Hydrogen shows noticeable permeation, even though its molecule is larger than helium. The mechanism of this anomalous observation is proposed and later corroborated by experiments. To make the generally “impermeable” graphene not only “permeable” but also highly “selective”, we have developed a perforation technique which involves a short-time exposure of the graphene membrane to low-energy electrons. Using the same monocrystalline containers, we are able to study gas transport through the created individual graphene pores with an effective size of about one missing carbon ring. Helium and hydrogen permeate easily through these pores whereas larger molecules such as xenon and methane are blocked. Permeating gases experience activation barriers that increase quadratically with the kinetic diameter, and the transport process crucially involves surface adsorption. Following these studies and to move a step further toward angstromporous 2D membranes with a high density of pores, other 2D membranes including graphene oxide and monolayer titania were made and their molecular and ionic transport properties were measured.

References:

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- [2] P. Z. Sun, et al. *Nat. Commun.* 2021, 12, 7170.
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Comparing Transport in Carbon-Nanotube, Boron-Nitride-Nanotube and Heterostructured-CNT-BNNT Membranes

Authors: Semih Cetindag, Da-Chi Yang, Richard J. Castellano, Pavel Rehak, Robert F. Praino, Liping Liu, Shigeo Maruyama, Petr Kral, Francesco Fornasiero, Sangil Kim, Jerry W. Shan

Affiliation: Rutgers University

Abstract: We seek to develop insight into some of the fundamental mechanisms underlying nanofluidic transport by comparing water and ion transport in different nanotubes. Using a solution-based, field-assisted method that is simple and flexible with respect to the types of nanotubes that can be used, we have fabricated macroscopic membranes with vertically aligned carbon-nanotube (CNT) or boron-nitride-nanotube (BNNT) pores. We have also fabricated axial BNNT-CNT heterostructures by coating vertically aligned single-wall CNTs (SWCNTs) with a few layers of hexagonal boron nitride (h-BN). We find that few-nanometer-diameter CNTs have large hydrodynamic slip lengths and marginal ion selectivity, while BNNTs of similar size have negligible slip lengths but are highly ion selective. Ion transport in such BNNTs is not only enhanced with respect to bulk, but also shows unexpected selectivity between different monovalent cations. Under either osmotic pressures or electric fields, BNNTs show enhanced (4-7-fold) transport rates for Li^+ over other alkali-metal ions (K^+ and Na^+) that are opposite to the ordering of their bulk mobilities in solution. As a result of the enhanced, selective transport, the BNNTs showed osmotic-power densities up to $15,300 \text{ W/m}^2$ for 1M:1mM LiCl at pH=11, while the CNTs of similar size showed negligible osmotic power generation. Thus, despite their identical crystallographic structure and diameter, few-nanometer-diameter CNTs and BNNTs have very different water and ion-transport characteristics. Intriguingly, we also find that sub-nanometer-diameter CNTs display transport properties that are fundamentally different from few-nanometer-diameter CNTs. As a result of their extreme confinement and localized tip charge, very-small CNTs show ion selectivities and osmotic-power generation akin to that of larger BNNTs. Furthermore, we find that SWCNTs exhibit charge-regulation and hydrodynamic translucency. When externally coated with a few layers of h-BN, the SWCNTs showed greatly reduced hydrodynamic slip and increased surface charge and enhanced cation selectivity. This suggests that not only could the transport properties of nanotubes be tuned by engineered coaxial heterostructures, but that the choice of matrix material may influence the transport properties of nanotube membranes. Finally, we summarize the different mechanisms affecting water and ion transport indicated by these observations, and discuss their possible implications for optimizing hydrodynamic transport and ion selectivity for diverse applications such as water filtration, energy conversion, and molecular separations.

Quantum Effects in Nanofluidic Transport: From Electrons to Ions

Authors: Tuan Anh Pham

Affiliation: Quantum Simulations Group, Lawrence Livermore National Laboratory, Livermore, California USA

Abstract: Quantum interactions become decisive in nanofluidic transport when water and ions are confined to molecular length scales. In this talk, I will highlight our recent simulation efforts to connect electronic-structure physics to the transport of water and ions under confinement. I will describe how we combine electronic-structure theory with machine-learned potentials and enhanced-sampling methods to access complex, reactive transport processes at nanoscales. We show that confinement and interfaces strongly reshape electronic polarization, hydrogen-bond structure, and electrostatic fluctuations across diverse material platforms—from carbon nanotubes to two-dimensional channels such as boron nitride—thereby renormalizing dielectric screening relative to bulk and altering the free-energy landscape for ion solvation and transport. I will also discuss the role of nuclear quantum effects in water flow through carbon nanotubes, where subtle changes in the hydrogen-bond network measurably impact transport. I will conclude with an outlook on quantum-mechanical and quantum-informed approaches needed to model nanofluidic physics at realistic length and time scales.

A Multiscale Framework for the Analysis of Nanobubbles in Nanoconfined Domains

Authors: Peter Berg^{1,2}, Ali Ghamartale¹, Ehsan Shahini¹, Aditya Jain², Jiabin Wang¹, Mahnaz Sababkar¹, Mostafa Hosseini¹, Rogerio Manica¹, Tian Tang¹

Affiliation: ¹University of Alberta, Canada; ²Delhi Technological University, India; ³Brock University, Canada

Abstract: Nano-sized gas bubbles are gaining attention in electro-chemical applications due to their exceptional stability and impact on reaction kinetics. Controlling bulk or surface nanobubble formation inside nano-confined domains may even lead to new nanofluidic memory devices.

This research presents a multiscale framework combining molecular dynamics (MD) simulations and macroscale thermodynamic modeling to study nanobubble stability and shape under isothermal-isobaric condition. MD simulations are performed for hydrogen in water under supersaturation, and the results are compared with theoretical predictions from continuum theory.

Our findings reveal that nanobubbles form only above a critical gas supersaturation threshold and exhibit remarkable stability across a wide range of concentrations. Using MD simulations of a pure gas, van-der-Waals parameters are extracted which demonstrate that a real-gas model is essential for accurately predicting the extremely high pressures inside nanobubbles. We further demonstrate that the Young-Laplace equation holds even at sub-10 nm scales, with a negligible Tolman length.

Inspired by experiments, a special focus lies on surface nanobubbles inside cylindrical nanochannels, including their shapes and contact angles as a function of bubble size and diameter of the cylinder. Under hydrogen reduction, nanobubbles can form and last a long time even without further hydrogen evolution, dissolving again under hydrogen oxidation, effectively representing a binary memory device. Future work will investigate the associated timescales of formation, lifetime, and controlled dissolution.

Synergistic Nanofluidics Between Soft and Hard Condensed Matter

Authors: Alessandro Siria

Affiliation: Center for Advanced Nanoscale Functionalities (CANF), College of Physics and Optoelectronic Engineering, Shenzhen University, 518060 Shenzhen, China

Abstract: Carbon nanomaterials exhibit peculiar properties in terms of water permeation, ultra-low hydrodynamic friction, and enhanced ionic transport. These observations challenge the classical description of water-carbon friction and highlight the importance of interactions between the electronic properties of the confining solid and the behavior of fluids at the nanoscale. Recent advances now make it possible to directly couple electronic degrees of freedom in the solid to fluid flow and ionic transport, opening new routes to control nanofluidic phenomena. In this talk, we revisit the current state of the art in fluid transport at the nanoscale and present recent experimental investigations of the complex coupling between fluid dynamics and the electronic properties of confining materials.

Opening the Black Box: Operando Microscopy Transforms Nanofluidics

Authors: Aleksandra Radenovic

Affiliation: Institute of Bioengineering, School of Engineering, Swiss Federal Institute of Technology Lausanne, Lausanne, Switzerland

Abstract: Nanofluidics has long promised transformative applications in biosensing, energy, and information processing, but progress has been limited by the difficulty of observing molecular transport in confined geometries in real time. Operando microscopy is now changing this landscape. By coupling high-speed, single-molecule-sensitive imaging with electrical, mechanical, and optical probes, we can directly watch how ions, biomolecules, and even quantum emitters behave inside nanofluidic devices. This ability to visualize transport and structural transitions as they occur is revealing unexpected mechanisms—such as electromechanical blistering in 2D channels, lumen-charge-controlled gating in protein pores, and liquid-activated emission in hBN that underpin new generations of robust sensors and ionic memristors. In this talk, I will show how operando microscopy is transforming nanofluidics from a “black box” discipline into a design-driven science, enabling reproducible device architectures, scalable iontronic circuits, and entirely new modes of quantum and molecular sensing.

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Next-Gen 2D Membranes with Ordered, Atomically Precise Channels

Authors: Jie Shen

Affiliation: School of Materials Science & Engineering, Nanyang Environment & Water Research Institute (NEWRI), Nanyang Technological University

Abstract: Biological channels can efficiently and selectively transport water, specific ions, or molecules, owing to the uniform sub-nanometer (sub-nm) pore diameters and unique surface chemistry of protein channels (Ref. 1). Creating artificial channels with similar structures and functions and developing their membranes have profound implications for energy-efficient separations in applications ranging from water purification to petroleum refining, chemicals production, and carbon capture (Ref. 2). 2D materials with atomic thickness and large lateral dimensions offer great opportunities to create membranes that can theoretically afford ultimate permeation properties. However, the practical development of 2D materials membranes for sub-nm scale separations is hindered by some critical challenges, including the controlling of non-selective defects and channel size distribution, and long-term stability under industrial-like conditions.

In this talk, I will present strategies for designing and tuning 2D materials channels and their mass transport behaviors at the sub-nm scale, including selective transport of gas, liquids, and ions as separation membranes. These include making ordered interlayer channels (*Angew. Chem. Int. Ed.*, 2015; *ACS Nano* 2016) and controlling the interlayer size and chemistry (*Nature* 2017; *Adv. Funct. Mater.* 2018). In contrast to the previous efforts using uncontrollably drilled holes in 2D layers, we demonstrate nanometer-thick 2D polymer membranes (*Nat. Mater.* 2022) and monolayer MoS₂ (*Science* 2025), which intrinsically had sub-nm in-plane pores that are robust and highly selective to water.

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Angstrofluidics in 2D Molybdenum Disulfide Channels

Authors: Heechan Yang, Sangyeon Jo, Sangyeon Lee, Hyung Gyu Park

Affiliation: Nanoscience for Energy Technology and Sustainability (NETS), Department of Mechanical Engineering, Pohang University of Science and Technology (POSTECH), Pohang, Gyeongbuk 37673, Republic of Korea

Abstract: A single-angstrom-digit space provides a fundamental basis for the efficacy and efficiency of transmembrane protein channels, thereby engendering a prime area of study in nanofluidics. We present the kinetics of water and ions in a two-dimensional (2D) molybdenum disulfide multichannel with a diameter of 3.1 Å. Water in tight 2D confinement can crystallize and move collectively, exemplifying structure-induced dynamics. Although the angstrom-level entrance incurs a severe energy penalty, such as dehydration, the surface charge enables the passage of ions, exhibiting a Hillian isotherm similar to the biophysical mechanism found in biochannels. Our findings on molecular conduction in a 2D confined environment reveal new insights and the potential that Angstrofluidics promises to unlock.

Breakdown of Conductance Scaling in Atom-Scale Artificial Ion Channels

Authors: Chih-Yuan Lin¹†, Rachael N. Keneipp¹†, Pia Bhatia¹, Trey T. Shin¹, George Siokos¹, Alexandra Sofia Uy-Tioco², Adrien Nicolai³, Marija Drndić^{1*}

Affiliation: ¹Department of Physics and Astronomy, University of Pennsylvania; Philadelphia, PA, 19104, USA; ²Department of Materials Science and Engineering, University of Pennsylvania; Philadelphia, PA, 19104, USA; ³Université Bourgogne Europe, CNRS, Laboratoire Interdisciplinaire Carnot de Bourgogne ICB UMR 6303, 21000 Dijon, France

Abstract: Ion transport in artificial channels that mimic biological ion channel behavior would enable advances in neuromorphic computing and biomolecular sensing. We fabricate atom-scale artificial ion channels in multilayer hexagonal boron nitride (hBN) and demonstrate a new regime of ion transport. Channels ranging from 0.5 to 1.5 nm in diameter reveal unconventional ion transport under conditions of extreme confinement: the conductance G remains approximately constant regardless of bulk ion concentration c and is significantly enhanced as c decreases. Molecular dynamics simulations support this G versus c relationship, suggesting a single-file ion transport mechanism without dehydration. Post-measurement characterization shows the stability of our hBN channels, ensuring experimental reliability. These findings open new avenues for understanding ion transport phenomena in artificial ion channels at the atomic scale.

Experimental Demonstration of Ambipolar Ion Transport with Ratchet-Based Ion Pumps

Authors: Karen Shushan¹, Alon Herman¹, Dafna Amichay¹, Eden Grossman¹, Ilan Bijaoui¹, Ras Samira¹, Rahul Saxena¹, Baruch Hirsch¹, Brian Rosen², Gideon Segev¹

Affiliation: ¹School of Electrical Engineering, Tel Aviv University, Tel Aviv 6997801, Israel; ²Department of Materials Engineering, Tel Aviv University, Tel Aviv 6997801, Israel

Abstract: Even though highly selective ion pumps are found in the membrane of every living cell, artificial ion selective separation is a longstanding unmet challenge in science and engineering. Ratchet-based ion pumps (RBIPs) are membrane-like devices that utilize temporal potential modulation to drive a net ionic flux with no associated electrochemical reactions. Recent theory predicts that ratchet-based ion pumps can sort ions according to their diffusion coefficients and induce ambipolar transport—driving both anions and cations in the same direction. Here we report the first experimental demonstration of ambipolar ion transport with RBIPs.

RBIPs were fabricated by coating one surface of a nanoporous alumina wafer with gold and the other with platinum, forming an asymmetric nano-porous capacitor-like device. The electric field within the nano-pores is modulated by oscillating the capacitor voltage. Thus, when immersed in a solution, ions within the pores experience a modulating electric field resulting in ratchet-based ion pumping. The RBIPs performance was studied for various input signals, geometries, and solutions. RBIPs were shown to drive ionic current densities of several $\mu\text{A}/\text{cm}^2$ even when opposed by an electrostatic force. Ambipolar transport was verified by measuring the conductivity change between two compartments separated by the RBIP. RBIPs operated with signal amplitudes as low as 0.8 V drove an ambipolar K^+ , Cl^- ion flux of about $0.05 \mu\text{M}/\text{cm}^2\text{h}$ leading to a buildup of a 1.3 concentration ratio between the two compartments.

Chirality-Dependent Rare Earth Ion Transport and Separations in Carbon Nanotube Porins

Authors: Jobaer Abdullah^{1,2}, Yu Chen¹, Yuhao Li¹, Tuan Anh Pham¹, Aleksandr Noy^{1,2}

Affiliation: ¹Lawrence Livermore National Laboratory; ²University of California Merced

Abstract: Rare earth elements have been powering the key technologies shaping our societies, yet their production and availability are severely constrained by the lack of clean and efficient separation approaches. In this work we investigated the selectivity and efficiency of REE³⁺ ions transport through the inner pores of species-pure sub-1-nm diameter carbon nanotube porins (CNTPs). We report that REE³⁺ ions enter these extremely narrow pores and translocate through them with transport rates that are only an order of magnitude lower than that of K⁺ ions. CNTPs channels also exhibited statistically- significant selectivity between light and heavy REE ions. Surprisingly, semiconducting CNTP channels translocated REE ions consistently faster than the metallic CNTPs of the same diameter and also exhibited statistically significant discrimination between heavy REE ions. Density functional theory (DFT) simulations examined the microscopic mechanism of REE³⁺ ion entry into CNTPs, revealing that these ions translocate through the CNT channel as hydroxylated species.

Polyelectrolyte Brushes-Confined Nanofluidics

Authors: Ping Yu

Affiliation: Beijing National Lab for Molecular Sciences, Key Lab of Analytical Chemistry for Living Biosystems, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China; University of Chinese Academy of Sciences, Beijing 100049, China

Abstract: The behaviors of ion transport in confined channels are strongly related to the geometry and chemistry of channels. Polyelectrolytes are one kind of typical substrate with rich chemistry. By grown polyelectrolytes brushes onto the inner wall of micro/nanopipette by ATRP (atomically transfer radical polymerization), the polyelectrolyte brushes-confined nanofluidic configuration were successively and controllably obtained. With this configuration, several counterintuitive ion transport behaviors were observed, such as microscale ion current rectification, ion current rectification inversion for monovalent anions and ion current oscillation. Based on these fundamental behaviors, various sensors with high spatiotemporal resolution, especially for in vivo analysis, were developed. More recently, the hysteresis phenomenon was observed in polyelectrolyte brushes-confined nanofluidic. Typical three fingerprint characteristics of memristor were observed at polyelectrolyte-confined nanofluidic system. Moreover, the typical neuromorphic functions, such as PPF, PPD and dynamic filter properties were also realized. More importantly, chemical-related neuromorphic functions (i.e., chemical-electrical signal transduction) were for the first time accomplished, showing promising application in brain-mimic computing and brain-computer interfacing. We have also realized the neuron functions with polyelectrolyte brushed-confined nanofluidic with both electrical and chemical responsibility. We think the polyelectrolyte brushes-confined nanofluidic paved a way of tuning ion transport behaviors with rich chemistry and tunability, which would feature more diversity and tunability for the nanofluidic-related applications.

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Field Effects in Proton Transport through 2D Crystals

Authors: Marcelo Lozada-Hidalgo

Affiliation: The University of Manchester

Abstract: Graphene is impermeable to all atoms^{1,2} and ions^{3,4} under ambient conditions in the direction perpendicular to its basal plane, but is permeable to thermal protons⁵. This opened a long-standing debate on whether the proton permeability was intrinsic to the material or due to vacancies. Protons can also chemically adsorb on graphene and recent work demonstrated that this process can be driven electrochemically, triggering a robust conductor-insulator transition in graphene⁶, but its mechanism remains unknown. In this talk we'll discuss our recent work mapping proton transport currents in graphene with nanoscale spatial resolution, which unequivocally confirm that perfect graphene crystals are permeable to protons and settle the long-standing debate⁷. We will also discuss our work investigating the mechanism of the electrochemical hydrogenation of graphene and the role of corrugations and isotope effects in this process. We will then discuss our recent work on the selective acceleration of proton transport and hydrogenation in double-gated monolayer and twisted bilayer graphene⁸. Our main finding is that independent control of the charge density and the electric field in graphene enables the selective acceleration of these otherwise coupled processes. This represents a new way of driving electrochemical processes with applications in logic-and-memory devices and energy.

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Nanoporous Atomically Thin Membranes for Challenging Chemical Separations

Authors: Rohit Karnik

Affiliation: Abdul Latif Jameel Professor, Department of Mechanical Engineering; Director, Abdul Latif Jameel Water and Food Systems Lab, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge MA 02139, USA

Abstract: Nanoporous atomically thin membranes, wherein nanopores in a single layer of two-dimensional material such as graphene provide pathways for rapid and selective fluidic transport, constitute the thinnest possible membrane and have potential for improving the efficiency, selectivity, productivity, versatility, and chemical resistance for a variety of membrane separations. Through controlled nucleation of defects via ion bombardment and oxidative etching, sub-nanometer pores are created in a single layer of graphene placed on a porous support. We discuss strategies for the design of membranes that are tolerant of defects in the graphene layer, and show that appropriate choice of the porous support is critical for exploiting the selectivity of nanoporous graphene. We further demonstrate that the impermeability of graphene can be exploited to selectively seal defects to tighten the pore size distribution and functionalize the pores to improve its selectivity. Through these developments, we realize centimeter-scale graphene membranes for nanofiltration and dialysis, demonstrating ultrahigh permeance and Angstrom-scale molecular geometry-based selectivity in organic liquids, high-temperature hydrogen/hydrocarbon separations, and separation of metal ions such as lithium and rare earths. These studies illustrate the interplay between material structure and transport in nanoporous graphene and demonstrate its potential to realize versatile, tunable, and chemically-stable next generation membranes for chemical separations, resource recovery and recycling, and water purification to unlock industrial materials circularity and energy efficiency for a sustainable future.

Engineering Non-Equilibrium Electrostatics in Bipolar Nanopores

Authors: Joan M. Montes de Oca

Affiliation: Materials Science Division, Argonne National Laboratory, Lemont, Illinois 60439, United States; Advanced Materials for Energy-Water Systems (AMEWS) Energy Frontier Research Center, Argonne National Laboratory, 9700 South Cass Avenue, Lemont, Illinois 60439, United States.

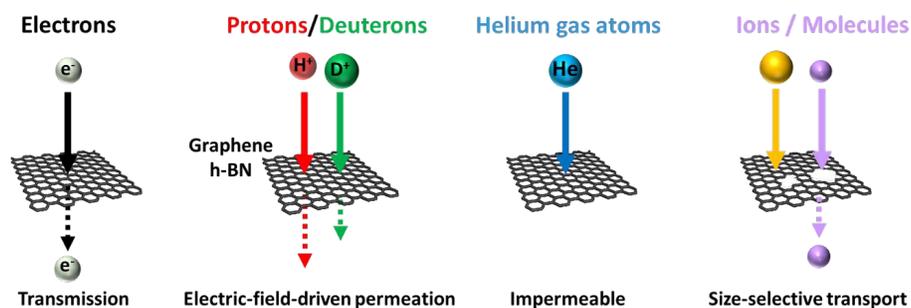
Abstract: Electrostatics is central to nanofluidics, yet most research has focused on equilibrium phenomena such as electric double layer overlapping in charged nanopores. Non-equilibrium effects, including electrically driven space charge formation, remain a comparatively untapped resource in nanofluidic systems. Here, we demonstrate how non-equilibrium electrostatics can be engineered in bipolar (Janus) nanopores and exploited as a design principle. Through a combined modeling approach of all-atoms molecular dynamics and continuum Poisson–Nernst–Planck calculations, we uncover the fundamental mechanism of space charge formation and its amplification under nanoconfinement. We show that engineered space charge enables strong ionic current rectification by modulating ionic concentration polarization. Furthermore, we demonstrate that these purely electrostatic effects can give rise to emergent device-like functions, including spiking and voltage-gated ionic currents, without any mechanical components. This work recasts non-equilibrium electrostatics as a main character in nanofluidic design, shaping iontronic devices, separations, and energy conversion technologies.

Atomically Thin Proton Exchange Membranes: Synthesis, Processing, and Device Integration

Authors: Piran R. Kidambi, Pavan Chaturvedi, Aman Tamboli, Peifu Cheng, Nicole Moehring,

Affiliation: Chemical and Biomolecular Engineering, Mechanical Engineering, Vanderbilt University

Abstract: Two-dimensional (2D) nanomaterials offer new opportunities to probe and control mass transport at the molecular and sub-nanometer scales. Their atomic thickness enables phenomena such as quantum tunneling and their ability to sustain defects that manifest as nanopores in an atomically thin membranes allow highly size-selective ionic/molecular sieving - opening new frontiers in separations. This talk will highlight our recent advances in the synthesis, integration, and scalable processing of 2D materials for electrochemical systems including proton exchange membranes for fuel cells, flow batteries, as well as other emerging separation applications such as hydrogen isotope sieving. Specifically, the talk will focus on Angstrom-scale proton selective pore-creation in atomically thin 2D materials along with the development of scalable integration pathways to realize next-generation PEMs that over-come the permanence vs selectivity trade-off in state-of-the-art conventional PEMs in fully functional applications.



Ion Permeability vs. Thickness: Fundamental Limitations and Curious Opportunities for Ultrathin Films

Authors: Viatcheslav Freger

Affiliation: Wolfson Department of Chemical Engineering, Grand Water Research Institute, Grand Technion Energy Program, Russel Berrie Nanotechnology Institute, Technion Israel Institute of Technology, Haifa, Israel

Abstract: Selective ultrathin membranes play key role in biology and osmotic membrane separations. The latter typically require a high permeability to water P_w and low salt permeability P_s achieved through strong exclusion in the low-dielectric films. Both P_w and P_s are commonly viewed as intrinsic properties, which is well justified for water, as its interaction with the membrane does not extend beyond closest neighbors. However, for ions, electrostatic interactions are long-range thus ion exclusion is affected by the proximity to high-dielectric surrounding in a thickness-dependent manner, as pointed out long ago by Parsegian. His analysis indicated that the Bjerrum length of the membrane, inversely proportional to its dielectric constant, should represent a limiting thickness, below which P_s sharply increases and selectivity drops.

While biological membranes are close to this limit, it has long been irrelevant for synthetic films. However, modern coating techniques such as molecular layer deposition (MLD) approach and surpass this limit. The progress in applying these techniques for membrane development motivates quantitative understanding of the relation between the film thickness and P_s . We rigorously derived such relation, using far more involved computations than semiquantitative Parsegian's analysis. Notably, the thickness-dependence of P_s , fully dictated by the Bjerrum length, may be factored out of the genuine intrinsic permeability P_∞ . This presents an attractive new opportunity for assessing the film's dielectric properties in working conditions. We demonstrate utility of this approach by applying it to (a) proton permeation in lipid membranes, 2 to 3.5 nm thick, and (b) MLD-synthesized polyamide films, 2 to 20 nm thick. Remarkably, the outcome is unrelated to P_∞ and, in fact, may help advance its understanding, still insufficient at present.

Mimicking Biological Ion Channels Using Voltage-Gated Graphene Nanochannels

Authors: Yahui Xue

Affiliation: Department of Mechanics and Engineering Science, Southern University of Science and Technology

Abstract: Biological ion channels acting as life's transistors can gate simultaneously fast and selective ion transport through atomic-scale filters to maintain vital life functions. However, the quest of artificial structures to mimic biological systems for medical, sensing and energy applications has been hindered in achieving simultaneous ion selectivity, fast transport, and electrical gating at atomic scale. Recent progress in atomic-scale ion transistor research from fundamental mechanisms to potential applications will be firstly introduced. The atomic-scale ion transistor made of graphene channels of 3 angstrom size achieves simultaneously ultrafast and highly selective ion transport controlled by electrical gating. The underlying mechanism is attributed to the highly dense packing of ions and their concerted movement inside the graphene channels. Inspired by the ultra-sensitive thermoelectric response of thermoTRP channels, boosted thermoelectric response in voltage-gated graphene nanofluidic channels will also be discussed. I will show that a voltage-gated nanofluidic synapse can also be developed based on atomic-scale graphene channels, which exhibits both short- and long-term plasticity. The cation- π interactions at graphene surface enable the nanofluidic synapse to exhibit ultra-long-term memory.

Rotating Helices in Nanoscale Pores

Authors: Aleksei Aksimentiev

Affiliation: Department of Physics, University of Illinois at Urbana-Champaign

Abstract: Flowing fluid past chiral objects has been used for centuries to power rotary motion in man-made machines. By contrast, rotary motion in nanoscale biological or chemical systems is produced by biasing Brownian motion through cyclic chemical reactions. Recently, we showed that a chiral biological molecule, a DNA or RNA duplex, rotates unidirectionally at billions of revolutions per minute when an electric field is applied along the duplex, with the rotation direction being determined by the chirality of the duplex [*Nature Nanotechnology* 18:238]. The rotation was found to be powered by the drag force of the electro-osmotic flow, realizing the operating principle of a macroscopic turbine at the nanoscale. Here, we show how unidirectional rotation of nanoscale helices can be driven by out-of-equilibrium conditions, such as temperature or particle concentration gradients. Further, we show that the rotation of a DNA duplex can move water and ions through nanoscale pores. While the rotation-induced flow of water is generated by the steric shape of the DNA molecule, an even faster transport of cations is caused by electrostatic interactions. The rotation-induced ion flux is found to depend on the cation type, offering potential utility for ion separation. Finally, we show that the torque-driven duplex can move ions against their concentration gradient, realizing the Archimedes screw principle at the nanoscale.

Frictionless Flow of Surface Ions in 2D nanopores

Authors: Kittipitch Yooprasertchuti¹, Yanwen Yuan¹, Tihomir Marjanović¹, Slaven Garaj^{1,2,3,*}

Affiliation: ¹Department of Physics, National University of Singapore, Singapore; ²Department of Biomedical Engineering, National University of Singapore, Singapore; ³Department of Materials Science and Engineering, National University of Singapore, Singapore

Abstract: Understanding ion and water transport through nanometer-scale constrictions—with surface morphology controlled down to the atomic level—is essential for elucidating biological channel behavior and designing next-generation active nanofluidic devices. We investigated pressure-driven ionic currents in individual nanopores fabricated in atomically thin and ultrasmooth WS₂ membranes. As the nanopore diameter decreased, we observed a pronounced and progressive deviation from the expected scaling relationship between streaming and electrophoretic currents predicted by classical models. Across a range of physical (pore size) and chemical (ion concentration, pH) conditions, the experimental data could not be reconciled with standard models, even when assuming unphysical values for surface charge density and slip length. To explain these anomalies, we propose a model based on frictionless sliding of adsorbed ions along the smooth membrane surface, which captures the observed transport behavior across all tested conditions.

These findings reveal a previously unreported mode of surface-driven ionic transport, opening new directions for designing low-dissipation nanofluidic systems, and rethinking interfacial transport in 2D-material-based devices.

Neuromorphic Ionic Computing in Droplet-Based Biomimetic Synapses

Authors: Zhongwu Li, Aleksandr Noy

Affiliation: Materials Science Division, Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory

Abstract: Ionic neuromorphic devices emulate key neural functions by coupling ion transport with memory, enabling energy-efficient, biologically inspired computation. We present two generations of aqueous droplet-based synaptic systems that implement neuromorphic functions through tunable ion transport. The first platform, droplet interface synapses (DIS), employs lipid bilayers at droplet interfaces to generate coupled memristive–memcapacitive behavior under voltage stimuli. DIS exhibits short-term plasticity, Hebbian learning, and associative conditioning, and supports classification and reinforcement learning via reservoir computing. Building on this, we introduce membrane ion channel synapses (MICS)—a class of nanofluidic memristors based on voltage-gated ion transport through gramicidin A channels embedded in droplet interface bilayers. MICS devices display enhanced memristive hysteresis arising from voltage-dependent channel formation and ion dynamics, enabling more biologically realistic and energy-efficient neuromorphic function. Together, our results demonstrate the evolution of droplet-based neuromorphic platforms toward scalable, biomimetic nanofluidic computing architectures.

Few and Far in Between: Probing the Structure-Selectivity Relationship in Membranes using Path Sampling Techniques

Authors: Amir Haji-Akbari, Brian Shoemaker, Omar Khalifa, Hessam Malmir, Manuel Lopez

Affiliation: Department of Chemical and Environmental Engineering, Yale University

Abstract: The ability of semipermeable membranes to selectively impede the transport of undesirable ions and molecules is key to many applications, from desalination and gas separation to biological membrane transport. For instance, membranes that are only permeable to water and reject most other solutes are used in water desalination. Designing more selective membranes requires characterizing the kinetics and mechanism of the transport of the species rejected by the membrane. The timescales associated with such processes, however, can be too long to be accessible to conventional MD simulations. Moreover, the driven nature of the underlying separation processes excludes the utilization of most traditional advanced sampling techniques. Finally, the separation of timescales between the transport of desirable species (such as water) and undesirable species (such as salts) will result in considerable changes in reservoir concentration throughout an MD trajectory, which can skew the kinetics and mechanism of transport in ways that are difficult to quantify and correct. Recently, we utilized [1] jumpy forward flux sampling (jFFS) [2], a path sampling technique developed in my group, and non-equilibrium MD to study pressure-driven ion transport through nanoporous graphitic membranes. Our approach addresses all these challenges. It not only allows us to accurately and efficiently estimate arbitrarily long mean first passage times in nonequilibrium filtration processes, but also to compute fluxes and permeabilities within a pseudo-equilibrium ensemble in which both reservoirs are at different- but almost constant- chemical potentials.

In this presentation, I will first discuss several technical aspects of this new approach, particularly a new model that we have developed to correct for the rather strong finite size artifacts in simulations of non-equilibrium ion transport [3-4]. What is remarkable about this model is that it rectifies finite size effects “on the spot”, i.e., from the information obtained from a single finite simulation. Therefore, the behavior of the system in the thermodynamic limit can be inferred without a need to conduct multiple simulations of systems with different sizes (as is the common practice in the computational chemistry community). In addition, I will showcase several recent applications of this methodology to probe the physics of nanoscale ion transport, such as proximity-induced pore-pore correlations due to ion-dipole interactions [5], the anomalous dependence of ionic flux on pore length due to hydrophobic evaporation [6], and exploration of realistic membranes, such as biological channels.

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Nanofluidics beyond the Wall

Authors: Nikita Kavokine

Affiliation: The Quantum Plumbing Lab (LNQ), École Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

Abstract: Nanofluidic transport has traditionally been described with continuum equations, where the confining wall plays the role of a mere boundary condition. Yet, an increasing number of experiments falls beyond such descriptions, and point to the importance of the internal dynamics of the channel wall in determining its transport properties. I will discuss my lab's ongoing effort to develop a "Nanofluidic Standard Model" – an overarching framework, beyond continuum equations, that puts all the relevant degrees of freedom in the fluid and in the channel wall on equal footing. Among other examples, I will show how our Standard Model outlines possible mechanisms for the anomalously large water slippage in carbon nanotubes.

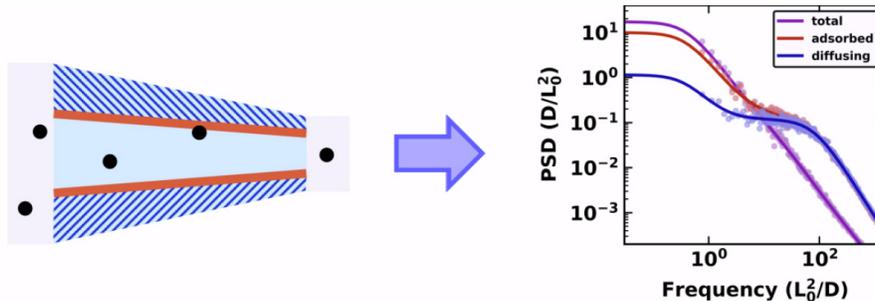
Decoding Noise in Nanofluidic Systems: Adsorption vs Diffusion Signatures in Power Spectra

Authors: Anna Drummond Young, Alice L Thorneywork, Sophie Marbach,

Affiliation: University of Oxford (ADY, ALT) Sorbonne Université (SM)

Abstract: Diffusive and adsorption processes play fundamental roles in molecular transport through nanofluidic systems, but in measured signals their signatures are hard to distinguish. At equilibrium, both processes affect the number of particles in a channel over time. The power spectral density (PSD) can quantify these number fluctuations and reveal key timescales linked to particle transport. While particle transport in channels has been studied theoretically via the PSD in the purely diffusive [1, 2] and purely adsorptive [3] cases, the coupling between both effects has been more rarely studied.

In this work [4], we derive an expression for the number fluctuations of particles diffusing in a channel, incorporating adsorption to the walls. We calculate the correlation functions and PSDs of the particle number fluctuations in the channel. Brownian dynamics simulations verify our theoretical predictions. The PSDs show characteristic scaling laws which emerge from specific physical mechanisms in the system; hence we can distinguish the effects of adsorption and diffusion. Notably, when there is a separation of diffusive and adsorptive timescales, the PSD can exhibit two distinct slopes. In general, contributions to the PSD from fluctuations in adsorbed and free particles are non-additive. We are currently applying our results to noisy data on polymer adsorption from in-house nanopore experiments.



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Effect of Flow Conditions on Electricity Generation at Interface Between Graphene and Flowing Water in Fluidic Channel

Authors: Takeru Okada¹, Mitsuhiro Honda², Masaki Tanemura², Ichiro Yamashita³, Atsuki Komiya⁴

Affiliation: ¹Graduate School of Engineering, Tohoku University, Japan; ² Department of Physical Science and Engineering, Nagoya Institute of Technology, Japan; ³ Graduate School of Engineering, Osaka University, Japan; ⁴ Institute of Fluid Science, Tohoku University, Japan

Abstract: The conversion of water current to electrical current through graphene has gained interest in both basic physics and applications such as electricity generation systems. Although various mechanisms have been proposed to explain this phenomenon, the general theory remains unclear. In particular, these mechanisms often do not consider the fluid conditions, including disturbance, irregular, and laminar flow conditions. In this study, we investigated the correlation between the flow conditions of flowing liquid water and generated electricity in graphene through experiments using several types of fluidic channels and numerical calculations.

Results suggest that the electricity output performance cannot be determined by the Reynolds number but by the local flow condition in the fluidic channel. In addition, the necessary condition for electricity generation is that the flow must be neither irregular nor laminar; instead, graphene responds to the transition process of the fluid [1]. Thus, the location of the graphene in the fluidic channel must overlap with the flow transition region from irregular near the inlet to laminar at the downstream in the channel, which enhances the interaction between the fluid and graphene.

Our findings support the extension of current theories and provide valuable insights into basic science in nano fluidic field and industrial applications.

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Nanopores with Dynamic Pore Opening Diameter for the Design of Ionic Memory Systems

Authors: Zuzanna S. Siwy

Affiliation: Department of Physics and Astronomy, University of California, Irvine, California 92697, United States; Department of Chemistry, University of California, Irvine, California 92697, United States

Abstract: I will present general design principles of nanopores which exhibit ionic memory that mimics how memories are stored in the brain. First, I will describe single nanopores drilled through a 10 nm thick gold layer positioned on top of a 30 nm thick silicon nitride film. The gold layer was modified with DNA using thiol chemistry. When an external electric field was applied across a nanopore with single stranded DNA, the nanoconfined DNA molecules exhibited steric and electrical constraints that led to memristor-like behavior in the current-voltage curves. The degree of hysteresis was controlled by salt concentration, magnitude of voltage and pore diameter. Molecular dynamics simulations revealed that the DNA played a role of electromechanical gate with voltage polarity dependent response. The second type of nanopores that will be presented store ionic memory in the frequency of ion current oscillations and fluctuations. When exposed to solutions of a weakly soluble salt, conical nanopores exhibit transient formation of nanoprecipitates observed as oscillations in the transmembrane current. The characteristics of the switching between high and low conductance states depend on the direction of the voltage scan, with memory effects embedded in the frequency of the switching as well as probability of a pore to be in the open state. The pores exhibit conductive synaptic switching behavior and show promise for neuromorphic computing applications. These two systems provide the first steps towards preparation of non-equilibrium nanopore systems.

Theory of Friction for One-Dimensional Water Structures Moving through A Sub-Nanometer Carbon Nanotube

Authors: Andy W.C. Lau¹, Jeffrey B. Sokoloff^{1,2}

Affiliation: ¹Department of Physics, Florida Atlantic University; ²Physics Department, Northeastern University

Abstract: In this talk, we present a unifying theoretical framework that underpins the flow of water and ions in carbon nanotubes (CNTs) with diameters of the order of a nanometer. Previous molecular dynamics simulations show that under such circumstances, water forms one-dimensional water wires or hollowed cylindrical periodic structures. Since these structures are likely incommensurate with the nanotube, they exhibit very low friction, analogous to “superlubricity” in solids. This fact provides a qualitative explanation for the high flow velocity of water observed in sub-nanometer CNTs. Since the one-dimensional nature of these structures dictates that they do not exhibit long range order, they are not pinned by defects. We calculate the sliding friction arising from phonon excitation in nanotubes and in water structures, and show that it scales linearly with the sliding velocity, and the interfacial friction coefficient is consistent with the results of the molecular simulations. Next, we consider the effects of random defects in the water structures and show that they give rise to a friction that is largely independent of the sliding velocity, i.e., dry friction, and demonstrate, based on the Langevin equation for a particle subject to both dry and viscous friction, that our model can account for the water flow measured in experiments. Lastly, we argue that there is also dry friction for ions moving in CNT’s, and demonstrate that this provides a natural explanation for the breakdown of the Nernst-Einstein (NE) relation for an ion moving in a subnanometer CNT, as observed in recent experiments.

Water and Ions in Angstrom-Scale Channels Made from 2D Materials

Authors: Radha Boya

Affiliation: Condensed Matter Physics Group, National Graphene Institute and Photon Science Institute, The University of Manchester, Manchester M13 9PL, United Kingdom

Abstract: Angstrom-scale confinement fundamentally alters the structure, dynamics, and transport of liquids, giving rise to phenomena that are absent in bulk systems. Two-dimensional material based angstrom-scale fluidic channels provide a uniquely well-defined platform to explore these effects, combining atomic-scale control of channel height, with tunable channel walls and their dimensions. Using such angstrom-scale channels, we have revealed highly selective ionic and molecular transport, enhanced ordering of confined water, and non-linear ionic conduction emerging from strong confinement and interfacial interactions [1-6]. These behaviours enable functional nanofluidic devices, including ionic memory elements, neuromorphic response, quantum emitters with implications for fluidic computing [4], and sensing applications [5]. Beyond transport, angstrom-scale nanofluidics offers new opportunities to probe the fundamentals of confined liquids. In this talk, I will also discuss advances in spectroscopy of confined water, outlining our experimental approaches to directly access molecular structure, and interactions under extreme confinement. Together, these studies highlight angstrom-scale confinement as a powerful framework for both discovery science and functional device engineering.

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Mixed Ion Transport in Confined Nanochannels of Microporous Polymer Membranes

Authors: Yuewen Jia, Sui Zhang

Affiliation: Department of Chemical and Biomolecular Engineering, National University of Singapore

Abstract: Ion transport in environments with mixed ions is crucial for numerous real-world applications. However, most membranes suffer from reduced selectivity in the mixed ion environment. In this talk, we will introduce the concept of dual-nanoconfined channel in covalent organic frameworks (COFs) for superior mixed mono-/multivalent ion separation. By incorporating acidic functionalities into the pore wall and coupling with a suitable pore size in the COF membranes, multivalent ions interact strongly with the acidic groups. This shields the interactions of the wall with monovalent ions, leaves sufficient space for fast monovalent ion passage, and in the meantime blocks multivalent ions, creating ideal dual-nanoconfinement for mixed ion separation. Consequently, mixed $\text{Li}^+/\text{Mg}^{2+}$ ion selectivity exceeding 1,300 and mono-/trivalent ion selectivity over 9,000 is achieved. Molecular dynamics simulation and experiment with multiple ion pairs further confirm the mechanisms.

Tissue-like Jammed Emulsions: An Emerging Biomimetic Architecture Towards Defect-free Ion Channel-based Membranes

Authors: [Aida Fica](#), Samuel West, Ronald J. Vogler, Claire Baldus, Manish Kumar

Affiliation: University of Texas at Austin

Abstract: Biological ion channels exhibit extraordinary perm-selectivity, and their integration into artificial membranes has long been pursued to overcome the permeability–selectivity trade-off. Such biomimetic systems could greatly outperform current separation technologies, yet the full promise of channel-based membranes remains unrealized because most platforms suffer from defects that bypass channel selectivity. This motivates the search for alternative membrane architectures that can be scaled while preserving the advantages of biological channels.

Jammed Interconnected Bilayer Emulsions (JIBEs) offer a new platform for bilayer-based, tissue-like architectures. In this system, a water-in-oil emulsion formed with a bilayer-forming amphiphile yields droplets coated by monolayers that form droplet interface bilayers (DIBs) upon contact. Centrifugation accelerates DIB formation and removes excess oil, producing a dense, jammed network of billions of bilayers per milliliter.

We demonstrate that JIBE bilayers are compatible with the functional incorporation of membrane proteins, positioning this platform as a promising scaffold for biomimetic membrane technologies. The water-in-oil environment provides an intrinsic barrier to ion leakage, greatly reducing defect pathways. Leveraging this inherent defect-free structure we show that JIBEs allow highly selective ion transport, even for demanding monovalent–monovalent separations. Remarkably, the selectivity signatures observed at the single-channel level are preserved across the entire JIBE network, representing the first demonstration of a biomimetic membrane in which transport behavior arises solely from the embedded channels rather than defects in the supporting scaffold.

Pillararene Water Channels - Structural Determinants for Enhanced Filtration Performances in Bilayer and Polymeric Membranes

Authors: Mihail Barboiu

Affiliation: Institut Europeen des Membranes, ENSCM-UMII-UMR CNRS 5635, Place Eugene Bataillon CC047, 34095 Montpellier, France

Abstract: During the last years diverse Pillar[n]arenes have been intensively used as molecular systems for recognition and synthons for self-assembly, toward the construction of highly selective supramolecular materials or functional devices. They present an electron-rich cavity, as well as reactive rims that can be decorated with specific functional groups, resulting in the formation of tubular pillar shape architectures. For this reasons pillar[n]arenes are excellent candidates for the construction of artificial water, ionic, proton, or molecular channels through bilayer and polymeric membranes used for selective separations. This lecture integrate the most recent examples of pillar[n]arenes synthetic systems used to elaborate selective channels or nanodevices for selective water translocation, ion or proton rectification useful for important application in environmental sciences as water purification or medicine.

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Passage of Gases and Vapors through Nanoporous Two-Dimensional Carbon Nanomembranes (CNMs)

Authors: Yang Yang, Zhen Yao, André Beyer, Petr Dementyev, [Armin Götzhäuser](#)

Affiliation: Physics of Supramolecular Systems and Surfaces, Bielefeld University, Germany

Abstract: Research into the use of two-dimensional materials as nanoconduits for molecular transport and separation is gaining momentum. In this study, we present the fabrication and application of carbon nanomembranes (CNMs), which are approximately 1 nm thick and created through the electron-induced cross-linking of aromatic self-assembled monolayers. CNMs feature subnanometer pores with a density of approximately 10^{18} m^{-2} , equating to one pore per square nanometer. These membranes facilitate the rapid passage of water molecules while effectively obstructing the translocation of ions.

To investigate molecular transport through the complex sub-nanometer pores of CNMs, we examined the permeation of various gases and vapors, including D_2O , NH_3 , He, N_2 , O_2 , CO_2 , and C_4H_8 . Typically, molecular transport across membranes is expected to follow Arrhenius-like kinetics, where flux increases with temperature and decreases upon cooling. However, our temperature-variable permeation experiments, conducted between -50 and $+50$ °C, reveal an Anti-Arrhenius behavior for water and ammonia permeating through freestanding two-dimensional CNMs. Specifically, we observed that the permeation rate of water vapor significantly decreases with increasing temperature, while the transport of ammonia molecules increases markedly when the membrane is cooled to the dew point. Additionally, the liquefaction of isobutylene does not enhance its transmembrane flux. These findings will be discussed in relation to the principles of adsorption-controlled permeation.

Non-Monotonic Salt Dependence of Electro-Osmotic Flow in pH-Regulated Nanochannels

Authors: Mingyu Duan, Luanzhe Xu, Jiadong Chen, Guang Chen

Affiliation: Department of Advanced Manufacturing and Robotics, College of Engineering, Peking University, Beijing, 100871, PR China

Abstract: Electro-osmotic flow (EOF) in nanochannels exhibits a puzzling non-monotonic dependence on salt concentration, which contrasts with observations in microchannels and remains not fully understood. In this work, we address this phenomenon through a theoretical investigation of EOF in pH-regulated channels. New analytical approximations for electrostatic potential, EOF profile and electro-osmotic mobility beyond the Debye–Hückel limit are derived through asymptotic analysis. Our findings reveal that the surface electrostatic potential is independent of the channel size only when the half-channel size exceeds the Gouy–Chapman length. In contrast, surface ionization and net charge distribution play more crucial roles in EOF at the nanoscale, as they govern both the magnitude and the spatial distribution of the Coulomb driving force. As salt concentration increases, EOF velocity initially rises due to enhanced surface ionization, followed by a decline attributed to increased wall shear stress. This work provides key insights for EOF applications in nanofluidics and biomedical devices, and deepens the understanding of electrokinetic phenomena influenced by pH-regulation effects.

Key word: electro-osmotic flow, pH-regulated channels, asymptotic analysis

Part IV. Poster Abstracts

Interpore Coupling Effects on the Spreading Resistance of A Nanopore Pair

Authors: Jacob Bair, Thor Burkhardt, Zachery Gottshall, Matthias Kuehne

Affiliation: Department of Physics, Brown University

Abstract: Double-nanopore systems receive increasing attention for their use in advanced single molecule detection and characterization experiments and their potential applications in filtration and more efficient, label-free DNA sequencing [1-3]. In this work, we present an analytical model for the resistance of a two nanopores in series system, where the length of individual nanopores is considered small compared to the adjoining compartments. Comparing our model to finite element simulations, we find a radially non-homogenous current density distribution in the nanopores to yield a quantitatively better description of the spreading resistance as opposed to the assumption of a uniform density in the most relevant cases. We identify a coupling regime dependent on the length and radius of the central compartment and characterized by a deviation in the current density from the approximated form. From finite element simulations that include a finite surface charge density on the pores, we examine how the coupling regime is affected by the charge and compare it to an empirical description of larger effective pore sizes [4]. Our work provides criteria that allows for the better-informed design of nanopores in series devices for use in single biomolecule sensing experiments.

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Coupled Nanopore Devices Towards Advanced DNA and Protein Sequencing

Authors: Pia Bhatia, Chih-Yuan Lin, Kyril Kavetsky, Alexandra Sofia Uy-Tioco, Namrata Pradeep, George Siokos, Marija Drndić

Affiliation: Department of Physics & Astronomy, University of Pennsylvania, USA

Abstract: Single, solid-state nanopores have emerged as a robust platform for rapid detection and sensing of biomolecules. However, fast translocation speeds have kept direct sequencing of DNA and proteins out of reach. To this end, we fabricate a coupled nanopore system comprised of thin (~ 10 nm or less) silicon nitride pores stacked in proximity (~ 25 nm vertical separation) with a single 2D pore. 2D pores are drilled in either monolayer molybdenum disulfide (MoS_2) or ultra-thin (~ 5 nm or less) hexagonal boron nitride (hBN) via transmission electron microscopy (TEM) drilling. We demonstrate how this unique system can be used to detect long ($\sim 15,000$ base pairs) double stranded DNA (dsDNA), shown in Fig. 1. We also demonstrate detection of individual amino acids with our devices, using O-Phospho-L-tyrosine as a model analyte. Together, these data underscore the great potential of coupled nanopore systems in advanced biomolecular sequencing applications.

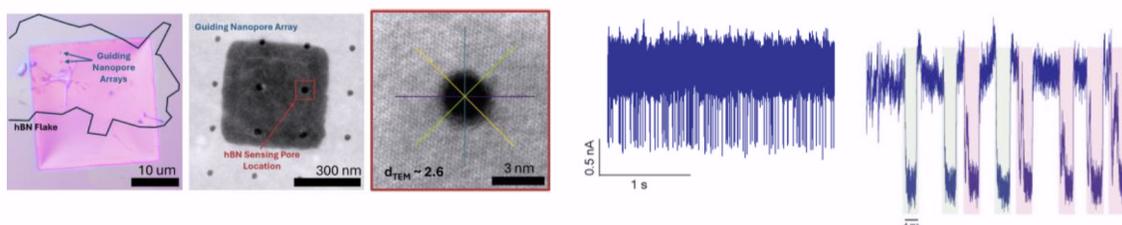


Fig. 1. Detection of 15K bp dsDNA in a coupled nanopore. From left to right: (1) Optical image of coupled nanopore device. (2) TEM image showing the guiding nanopore array, fabricated in a locally thinned region of silicon nitride (dark grey square). (3) TEM image showing a ~ 2.5 nm diameter pore in hBN, which is separated by ~ 25 nm from the SiN pore directly beneath. (4) Exemplary current trace obtained at 700mV, with 1MKCL. (5) Single and double-step events, colored in green and pink, respectively.

High-Dimension Ionic Memory in Oscillating Ion Current Signals

Authors: Anthony Dougman Cho¹, Agata Wawrzekiewicz-Jałowicka², Claudia E.P. Dewi³, Shiwei Tang¹, Ethan Cao¹, Craig Martens³, Tilman E. Schäffer⁴, Javier Cervera⁵, Patricio Ramirez⁶, Salvador Mafe^{5,7}, Zuzanna S. Siwy¹

Affiliation: ¹Department of Physics and Astronomy, University of California, Irvine, USA; ²Department of Physical Chemistry and Technology of Polymers, Silesian University of Technology, Gliwice, Poland; ³Department of Chemistry, University of California, Irvine, USA; ⁴Institute of Applied Physics, University of Tübingen, Germany; ⁵Dept. de Física de la Terra i Termodinàmica, Universitat de València, E-46100 Burjassot, Spain; ⁶Dept. de Física Aplicada, Universitat Politècnica de València, E-46022 València, Spain; ⁷Allen Discovery Center at Tufts University, Medford, MA, 02155-4243, USA

Abstract: Nanopores provide controlled nanoconfinement that can be utilized to induce localized chemical reactions. Here we present a nanopore exhibiting memory in the frequency of ion current oscillations induced by the dynamic formation and removal of nanoprecipitates within the pore volume. We find that the onset and characteristics of these current instabilities depend on the direction of the voltage scan, with memory effects evidenced in the frequency of switching between high and low conductance states, and probability of a pore to be in the open state. We have also emulated conductive synaptic switching behavior by applying voltage pulses, demonstrating the prospect of these nanopores for neuromorphic computing applications. A hypothesis is presented stating that the memory effects arise from the delayed formation and clearing of nanoprecipitates due to a spatial-temporal asymmetry, as well as long term variations in the effective surface charge. We also propose a model where precipitate formation is limited by the cation arrival rate. Our delayed logistic expression successfully recreates steady state and oscillatory features in the transmembrane current. The nanopore with memory encoded in the frequency of ion current oscillations emulates how brain stores memory and opens up a possibility for high-dimensional ionic memory for iontronics.

Enhancing Conductance of Two-Nanopore Arrays using Dual-Barrel Nanopipettes with Individual-Pore Electrochemical Tunability

Authors: Claudia E. P. Dewi, Anthony D. Cho, Kelly L. Vernon, Cody W. Leasor, Lane A. Baker, Tilman E. Schäffer, Zuzanna S. Siwy

Affiliation: University of California, Irvine

Abstract: In an effort to develop neuromorphic ionic devices, nanofluidics research has focused on investigating nanopore interactions. To realize high-density iontronic circuits, it is imperative to study the crosstalk between nanopores in an array, which is highly influenced by the interaction of ion concentration polarization regions. Our group has observed an ion conductance suppression resulting from overlapping depletion zones and predicted an enhancement when two closely-neighbor pores carry a surface charge of the opposite polarity. Verifying this prediction using a membrane-like nanopore array system is difficult due to the inability to probe individual pores. Therefore, we utilize a simple two-nanopore array system using quartz dual-barrel nanopipettes with a small interpore spacing necessary for the overlapping of ion concentration polarization regions to occur. This system permits several probing configurations of the array, including ion current measurements of the individual pores and both pores connected in series and parallel. Experiments performed in a wide range of KCl concentrations reveal a threshold concentration when two nanopores of the same surface charge connected in parallel show a sub-additive current. We will also show measurements and modeling where one pore is positively charged and the other one remains negatively charged. Multi-pore nanopipettes where each nanopore can be addressed electrically and chemically provide a unique tool not only to understand interactions between nanopores but also create ionic circuits.

Engineering Synthetic Macrocycles for Selective Rare Earth Elements Separation

Authors: Jiachen Feng, Martin Conda-Sheridan, Yuhao Li, Aleksandr Noy

Affiliation: Lawrence Livermore National Laboratory

Abstract: Rare earth elements (REEs) are critical components in advanced technologies that are notoriously difficult to separate due to their similar chemical properties. This study explores the design and use of a series of synthetic macrocycles to achieve selective lanthanide separation in a membrane configuration. We synthesized a series of macrocycles that integrate into lipid bilayers and demonstrate distinct variations in ion permeability attributed to differences in structural flexibility and specific functional groups. Notably, one of the macrocycles exhibits a six-fold difference in permeability between neodymium and dysprosium ions, underscoring its potential for selective REE separation. This work advances the understanding of macrocyclic ligand design, highlighting the balance between molecular rigidity, conformational freedom, and chemical functionalization as key factors in enhancing the selective transport of REEs. Our findings pave the way for more sustainable and efficient methods in lanthanide separation, potentially reducing dependence on traditional, less eco-friendly processes.

Formulation and Validation of A Nanoconfined Equation of State using Thermally Driven Isobars Within Single Digit Nanopores

Authors: [Sanjay S. Garimella](#)¹, Yu-Ming Tu², Rahul P. Misra¹, Lukas Arcuri³, Samuel Faucher¹, Matthias Kuehne⁴, Cody L. Ritt^{1,5}, Joshika Chakraverty¹, Xintong Xu⁶, Hananeh Oliaei⁷, Arun Majumdar⁶, Narayan Aluru⁷, Daniel Blankschtein¹, Michael S. Strano¹

Affiliation: ¹Massachusetts Institute of Technology; ²National Taiwan University; ³Technical University of Munich; ⁴Brown University; ⁵University of Colorado, Boulder; ⁶Stanford University; ⁷University of Texas at Austin

Abstract: The promise of next-generation water purification and separations devices is highly dependent on the precise tuning of fluid behavior in nanoscale pores. Although adsorptive processes within porous media have featured heavily in recent chemical engineering innovation, including pressure-driven distillation, there is no experimentally validated, predictive equation of state (EOS) for fluids subjected to nanoconfined volumes. We formulate and validate the first of such EOS using the interior of carbon nanotubes (CNTs) of precise diameters from 0.72 to 1.64 nm subjected to variable laser heating. We measure the interior density using the vibration of the encapsulating graphene wall, based on the radial breathing mode, to map the phase behavior versus temperature from ambient to over 600 K. The resulting traces of density versus temperature at constant pressure, or isobars, are well described by a confined fluid equation state, which builds on the work of Travalloni et al. Isobars are measured and described even in the limit of single file water for a CNT. Reformulating the EOS for a 2D geometry is able to predict the well-known maximum in capillary pressure at 1.3 nm spacing for a rectilinear graphene pore. We also find that for water, the enthalpy versus entropy of confined adsorption exhibits a linear compensation, similar to well-studied compensation effects in protein and kinetics literature. The validation of this EOS for nanopore systems is a significant advance in engineering prediction for the narrowest and technologically important materials.

Electronic Friction in Single-Digit Carbon Nanotubes and Quantum Osmosis

Authors: Peter Gispert, Hao Lu, Nikita Kavokine

Affiliation: The Quantum Plumbing Lab (LNQ), École Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

Abstract: In nanofluidics there is growing evidence for electronic couplings between the channel wall and the liquid. However, a solid theoretical understanding, in particular for single-digit (sub 10 nm diameter) nanotubes, is still elusive. My talk is based on the theoretical framework of quantum friction, which describes a van der Waals-type interaction between charge fluctuations of both materials. I will present a generalization of the quantum friction framework for cylindrical tube systems applicable to even the smallest carbon nanotubes. Based on that, I will show how electrolyte transport through the tube is sensitive to the tube metallicity, and even to the quantum phenomenon of van Hove singularities in the tube's band structure. Furthermore, I will present first experimental results for the inverse quantum friction effect, dubbed quantum osmosis, at the microfluidic water-metal interface, where an electronic current in the metal induces a water flow. These findings illustrate the complex electronic coupling of the channel wall with the liquid flow, paving the way to nanoscale electronic pumping and energy harvesting from water flows.

Ratcheting Up Selectivity: A New Paradigm in Ion Separation

Authors: [Alon Herman](#)¹, Joel W. Ager^{2,3}, Shane Ardo⁴, Gideon Segev¹

Affiliation: ¹School of Electrical Engineering, Tel Aviv University, 6997801, Israel; ²Department of Materials Science and Engineering, University of California at Berkeley, Berkeley, CA, 94720, USA; ³Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA; ⁴Department of Chemistry, Department of Chemical & Biomolecular Engineering, Department of Materials Science & Engineering, University of California Irvine, Irvine, CA, 92697, USA

Abstract: Water contamination has become a critical environmental problem, and a major health concern in many parts of the world. Current ion-filtration technologies cannot effectively remove low concentration contaminants, while keeping the minerals necessary for drinking water. As a result, highly selective membranes are becoming increasingly important.

Ratchet-Based Ion Pumps (RBIPs) are based on a flashing ratchet mechanism which utilizes modulations of a spatially asymmetric electric field to drive a steady state current. Using Ratchets' unique ability, the frequency dependent velocity reversal, it is feasible to drive ions with the *same* charge but different diffusion coefficients in *opposite* directions. This offers a new paradigm for ion separation, as same-charge ions can be perfectly separated directly at the membrane, without needing to travel long distances for high-precision separation.

Our simulations demonstrate effective separation, even with minimal diffusion coefficient differences (<1%), with separation ability directly proportional to this difference.¹ For example, when extracting Li^+ from a mixture of Na^+ and other common water-based cations, separation velocities can reach up to 3.6 cm/s. Since the pumping properties are determined by an electric signal, target ions can be tuned in real-time, enabling fit-to-purpose selective ion separation systems.

On a recent study we presented a feasible design for a multi-layered membrane with alternating electrodes in an asymmetric structure.² The model demonstrates that the multi-layered RBIP drives a net *ambipolar* ion flux (both cations and anions in the same direction), overcomes large concentration gradients (>100:1), and achieves frequency-dependent velocity reversal under realistic conditions. These capabilities make the membrane a promising candidate for distributed water desalination and high-selectivity applications like lead extraction from groundwater, where contaminants are at low concentrations.

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Control of Li Transport and Heterogeneous Charge Transfer Using Dual Electrolyte Gating

Authors: Eli Hoenig, Marcelo Lozada-Hidalgo

Affiliation: University of Manchester

Abstract: Understanding and controlling ion-electron coupling at solid-liquid interfaces is central to electrochemistry, energy storage, and nanoscale transport, yet remains challenging due to the entanglement of interfacial reaction driving forces, kinetics, and electrostatic gating. Here we employ a dual electrolyte-gated platform based on suspended (2D) materials that enables independent control of carrier density and electrochemical driving force. First, we study Li⁺ transport and insertion, where dual gating enables independent control of Li accumulation and drift. By decoupling Li⁺ flux from electronic doping, we enable an effective and robust ionic transistor. Next, using ferrocene/ferrocenium (Fc/Fc⁺) as a model outer-sphere redox couple, we directly tune heterogeneous electron-transfer rates by electrostatically shifting the Fermi level of the 2D electrode while independently controlling the electrochemical overpotential. This reveals a strong, gate-dependent modulation of reaction onset. Together, these results establish dual electrolyte gating as a powerful and general strategy for controlling both heterogeneous charge transfer and ion transport in low-dimensional systems, with implications for batteries, electrochemical sensors, and tuneable membrane and electrode architectures.

Solid-State Nanopore-Informed Technique for Statistical Modeling of Single-Molecule Protein Folding

Authors: Sabine Hong¹, Kyril Kavetsky^{1,2}, Chih-Yuan Lin¹, Roger Yang³, Celia Morral¹, Marija Drndić¹

Affiliation: ¹Department of Physics and Astronomy, University of Pennsylvania, USA; ²Department of Material Science and Engineering, University of Pennsylvania, USA; ³Department of Physics, Columbia University, USA

Abstract: Solid-state nanopores are highly customizable platforms for characterization of biomolecular structure and dynamics, including DNA as well as other nucleic acids, peptides, and proteins. Using high-bandwidth amplifier technology, combined with sensitive ultra-thin Silicon Nitride nanopores, we can detect the ultrafast folding and unfolding of the multi-state folding heme protein cytochrome c while it is constricted by the pore. We analyze the shapes of the resistive pulses generated by protein translocation and find that changes in ionic current correlate to discrete configurational states. Then, we model the relative favorability of each configurational state transition. The results give insight into the structural reconfiguration dynamics in single, native-state proteins which are essential for assessing biological function and preparing analytes for single molecule protein sequencing. We also use the model to determine starting and ending state probabilities, which provide insight into the mechanisms for nanopore capture and translocation of single proteins. Furthermore, this nanopore-informed technique for statistical modeling of structural reconfiguration dynamics in single proteins can be applied to other multi-state folding proteins as well as the simulation of protein behavior at the mitochondrial membrane.

Demonstration of A New Ionic Conductance Regime in Extremely Confined Nanopores

Authors: Rachael N. Keneipp¹, Chih-Yuan Lin¹, Pia Bhatia¹, Trey T. Shin¹, George Siokos¹, Adrien Nicolai², Marija Drndić¹

Affiliation: ¹Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, USA; ²Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR CNRS 6303, Université de Bourgogne, 21078 Dijon CEDEX, France

Abstract: In this work, we demonstrate a new regime of ion transport in sub-nm diameter two-dimensional (2D) solid state nanopores. Pores are made in multilayer hexagonal boron nitride (hBN) via aberration-corrected scanning transmission electron microscopy (AC-STEM) drilling and range in size from 0.5nm to 1.2nm. AC-STEM with integrated electron energy loss spectroscopy (EELS) capabilities allows precise nanopore fabrication and atomic characterization before and after ionic measurements. The combination of ionic conductance, AC-STEM, EELS, and atomic force microscopy provide a broad suite of information about pore geometries and composition. The findings reveal unconventional ion transport behavior under conditions of extreme confinement. In the sub-nm pore diameter range, the relationship between conductance and ion concentration exhibits pronounced nonlinearity. The conductance is significantly enhanced as concentration decreases, in stark contrast to measurements of larger pores (8nm). Molecular dynamic simulations indicate that, in line with experiments, the scaling behavior relating conductance to concentration no longer holds in the sub-nm hBN pores. Atomistic simulations also imply that surface charge on the hBN pores, which exhibits potassium selectivity, may contribute to enhancing this phenomenon at the sub-nm scale.

Ion Transport in Nanoporous Membranes: The Effect of Pore Length and Chemistry

Authors: Omar Khalifa

Affiliation: Yale University; Lawrence Livermore National Laboratory

Abstract: In this work, we use molecular simulations and advanced sampling techniques to investigate ion and water transport under nanoconfinement, focusing on graphitic nanoporous membranes and metal–organic frameworks (MOFs). We first address methodological challenges associated with polarization-induced finite-size artifacts that frequently arise in molecular simulations of ion transport. These artifacts originate from spurious interactions between traversing ions and periodic images of other ions. In earlier work, we developed physics-informed model to account for such artifacts. Here, we uncover a more subtle class of artifacts arising from spurious interactions between traversing and non-traversing ions across periodic boundaries, which can distort the underlying physics by altering the spatial distribution of non-traversing ions within the membrane.

Simulating a sufficiently large box can evade such artifacts. After establishing the fidelity of our simulations, we investigate the effect of pore length on ion transport. We find that at very short length scales, increasing the pore length can paradoxically lead to faster ion transport. Moreover, water transport does not exhibit a classical monotonic dependence on pore length. Instead, at specific pore lengths, ion and water transport become coupled, resulting in a loss of ion–solvent selectivity.

Finally, we probe ion dynamics in MOF-based membranes by characterizing cage-to-cage transitions and the associated free-energy landscape. Using forward-flux sampling, we map ion translocations and estimate transition rates. We further demonstrate that MOF surface chemistry can induce ion–ion selectivity, leading to preferential partitioning of one ion species over another.

Iontronic Synaptic Behaviors of Nanopipettes

Authors: Jingyi Li¹, Peiyue Li², Junjie Liu³, Xubin Qiu², Pan Zhang², Xiaofeng Shan¹, Wei Wang², Zhigang Cai¹

Affiliation: ¹Peking University School and Hospital of Stomatology & National Center for Stomatology & National Clinical Research Center for Oral Diseases & National Engineering Research Center of Oral Biomaterials and Digital Medical Devices, Department of Oral and Maxillofacial Surgery, Beijing 100081, China; ²School of Integrated Circuits, Peking University, Beijing 100871, China; ³College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China

Abstract:

Novelty: The device successfully mimics the function of biological synapses and shows strong potential for communication with biological neural systems. Based on fully aqueous solution system and biocompatible device structure, the device exhibits bipolar conductance memory and emulates key neuromorphic functions, representing a significant step toward building artificial systems comparable to biological ones [1].

Background: In biological systems, synapse is the basic functional unit (Figure 1a). In our previous work, we have developed a nanofluidic artificial synapse consisting of a nanochannel connected to two microchannels. By selecting aqueous solutions and ionic liquids, these devices demonstrated promising synaptic performance [2-3]. However, due to limitations in their planar structural, interfacing with biological cells remained challenging. Patch-clamp

technique enables the detection of ionic currents at the single-cell level, primarily in excitable cells such as neurons and muscle cells (Figure 1b). By mimicking the structure of the patch clamp [4], this work proposes a nanofluidic biomimetic synapse based on nanopipettes, making it promising to interact with living cells. By selecting appropriate aqueous electrolyte solutions and specific cation-anion pairs, ion hysteresis is achieved. We have made efforts to bridge the gap in interfacing with biological cells by optimizing both the device structure and the composition of the electrolyte solutions.

Description of the New Method or System: In this work, a novel nanopipette artificial neural synapse device was proposed. The nanopipettes were fabricated from the borosilicate glass capillaries using a P2000 CO₂ laser puller. In the setup, 10 mM TBACl solution located inside the nanopipette and connected to the reference electrode, while 100 mM KCl solution located outside and connected to the working electrode (Figure 1c). These two electrolyte solutions form a liquid/liquid interface at the nanopipette tip. The voltage was applied and the total ionic current was measured via Ag/AgCl and Ag electrodes in the KCl and TBACl solutions, respectively. Scanning electron microscope was used to characterize the diameter of the tip. The nanopipettes with a diameter of approximately 80 nm were chosen (Figure 1d).

Experimental Results: The device demonstrates excellent cyclic repeatability over 20 current-voltage (I-V) sweeping cycles (Figure 2a). Under positive voltage, the current gradually increases during the forward scan and decreases during the backward scan. Notably, the backward-scan current is larger than the forward-scan current at the same voltage.

A similar current hysteresis is also observed under negative voltage. The magnitude of the ionic current is governed by the number of ions transfer through the nanopipette tip. As the scan rate

decreases, the hysteresis loop area progressively increases, accompanied by an enhancement in the peak current during the forward scan (Figure 2b). Reversing the polarity of the electrodes results in an opposite rectification behavior (Figure 2c). Under pulse voltage, the device conductance increases with positive pulses and decreases with negative ones.

Furthermore, higher pulse amplitudes lead to faster changes in conductance (Figure 2d). In summary, we present a novel ionic synaptic device based on nanopipette. The device structure is biocompatible and the I-V curves exhibit a rectifying hysteresis loop, demonstrating iontronic synaptic behavior. This device holds promise for future integration with biological cells.

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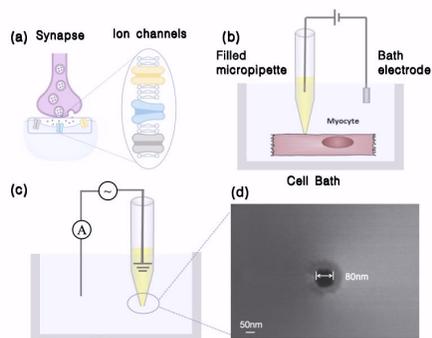


Fig. 1. (a) Schematic diagram of biological synapses as fundamental units mediating brain physiological functions. (b) The configuration of patch clamp. (c) Schematic diagram of the nanofluidic biomimetic synapse based on nanopipette. (d) Scanning electron microscope (SEM) image of the nanopipette tip (S4800, 3.0 kV, 8.4 mm, $\times 110k$, SE(M)).

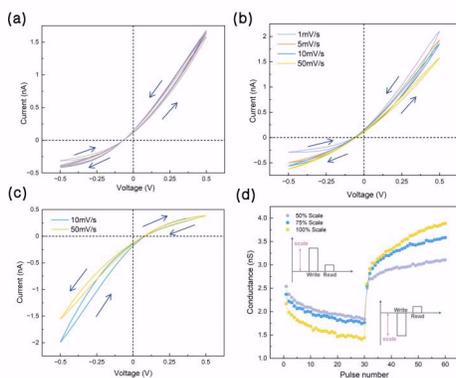


Fig. 2. Results of the experiment. (a) The 20 I-V sweeping cycles for the ionic synaptic device, the scan rate was 50 mV/s. (b) The I-V curves of the device at different sweeping rates, including 1 mV/s, 5 mV/s, 10 mV/s and 50 mV/s. (c) The opposite rectification behavior when the polarity of the electrodes are reversed, the scan rate was 10 mV/s. (d) Time-dependent conductance changes under various pulse amplitudes. The width of the voltage pulse was 200 ms, and a reference amplitude of 60 V and -2 V represents 100%.

Particle-gated, Ionically Driven Nanocantilever with Memristive Hysteresis in Liquid

Authors: Xinxin Liu, Göran Stemme, Frank Niklaus

Affiliation: Department of Micro and Nanosystems (MST), School of Electrical Engineering and Computer Science (EECS), KTH Royal Institute of Technology, Stockholm, Sweden

Abstract: Ions can actuate solids at the nanoscale. We show that an ultrathin inorganic nanocantilever in electrolyte develops a pinched, memristive I–V response when gated by a single nanoparticle. The device is an HfO₂ cantilever (5 nm thick; ≈ 50 nm \times 60 nm in size) as part of a nanofluidic pore. Upon adsorption of a 15 nm SiO₂ nanoparticle delivered from the bath, the current–voltage curve switches from single-valued to a pronounced self-crossing loop; in the particle-free state the I–V is non-hysteretic. Frequency-resolved ramps in aqueous KCl reveal a bell-shaped loop-area spectrum with a clear window of 0.05–5 Hz and a maximum near 0.7–1 Hz. The behavior is consistent with ionically mediated mechano-electrical coupling: asymmetric electro-osmotic shear and pressure around the adsorbed particle generate a net bending moment on the 5nm-thick cantilever, cyclically modulating the effective opening and thus the conductance. Ex-situ SEM confirms capture of the SiO₂ particle on the cantilever after biasing, directly linking the memristive state to particle occupancy.

To the best of our knowledge, this is among the smallest liquid-phase, ionically driven inorganic cantilevers, converting ionic transport into active mechanical actuation with purely electrical readout. The HfO₂ platform offers CMOS-compatible fabrication, nanometre footprints, predictable mechanics, and low-power operation, opening a path to particle-gated ionic memories and single-particle mechano-ionic sensors.

Keywords: nanofluidics; ionic memristor; electro-osmosis; nanocantilever; nanoparticle gating; pinched hysteresis

Electronic Correlations in 2D Materials Induced by Interfacial Water

Authors: Hao Lu, Nikita Kavokine

Affiliation: The Quantum Plumbing Lab (LNQ), École Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

Abstract: Interfaces between water and 2D materials have attracted widespread fundamental interest, due to their importance as building blocks for filtration membranes and energy storage systems. A growing number of experiments now points to the materials' electronic properties playing a role in the interfacial fluid dynamics. Yet, the usual density functional approaches only describe electronic properties at the mean field level, failing to account for strong correlation effects. Here, we study a model water-2D-material system using a quantum embedding approach that captures local correlations exactly. Our calculations reveal a water-induced polaron effect, corresponding to a slowdown of the electron dynamics as their motion correlates with water charge fluctuations. This results, in turn, in a slowdown of the interfacial water dynamics through an enhancement of the water-electron quantum friction. By combining a downfolding approach with dedicated molecular dynamics simulations, we extend our calculations to real material systems and reveal signatures of a polaron effect at the interface between water and niobium diselenide. Our results suggest that electronic correlations may be used to engineer nanoscale fluid transport and point to the importance of beyond-DFT approaches to solid-liquid interfaces.

Reversible Nanopore sealing via in situ Iron Oxide Synthesis

Authors: Celia Morral¹, Zehui Xia², Pia Bhatia¹, Brian DiPaolo², Chih-Yuan Lin¹, David Niedzwiecki², Iryna Golovina³, Marija Drndić¹

Affiliation: ¹Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA; ²Goeppert LLC, 3401 Grays Ferry Avenue, Philadelphia, Pennsylvania 19146, USA; ³The Laboratory for Research on the Structure of Matter, University of Pennsylvania, Philadelphia, PA 19104, USA

Abstract: We report in-situ synthesis of iron oxide particles (Fe_3O_4 and Fe_2O_3) inside silicon nitride (SiN_x) nanopores via a rapid chemical reaction between ferric, ferrous and hydroxide ions in electrolyte solution. The process is monitored by current readout and particles can be removed to recover pores. Pores range in size from 5 nm diameter to 60 nm diameter. We also study the dynamics of particle formation in nanopore arrays. Pores are characterized before and after iron oxide formation with transmission electron microscopy. We utilize energy dispersive X-ray spectroscopy, aberration-corrected scanning transmission electron microscopy, and powder X-ray diffraction to characterize the iron oxide we synthesize. We report the effects of reactant concentration, applied electric field, and pore diameter on particle formation. We also obtain a characteristic particle formation time to compare reaction kinetics across various pore sizes and concentrations.

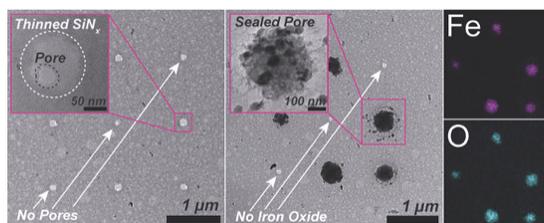


Fig. 1. TEM micrographs of nanopore array before and after iron oxide synthesis. EDS maps confirm the presence of iron oxide.

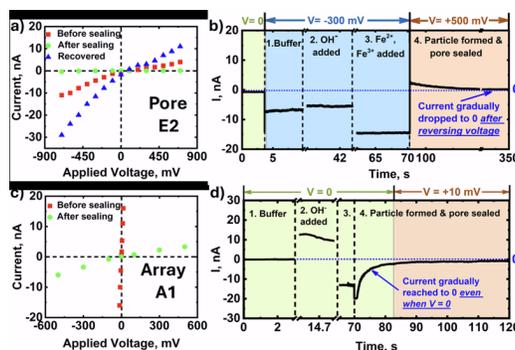


Fig. 2. IV curves for single nanopore (~ 6 nm diameter) and corresponding current trace during particle formation.

Measuring Nanoscale Flows with Quantum Sensing

Authors: Killian Rigaux, Nikita Kavokine

Affiliation: The Quantum Plumbing Lab (LNQ), École Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

Abstract: The permeability of a nanoscale channel is perhaps its most basic property, yet direct flow measurements remain an outstanding experimental challenge in nanofluidics. I will show that quantum sensing based on nitrogen-vacancy (NV) centers in diamond can be used to measure nanoscale flows. Our method relies on the ability of NV centers to detect magnetic noise in nanoscale volumes and on the difference of magnetic properties between water and heavy water. I will detail the principles and technical requirements for turning a NV sensor into a nanoscale flow meter and present proof-of-concept measurements at the microchannel scale. Given the exquisite sensitivity of NV centers, our method holds promise for detecting flows through the tiniest channels, such as single-digit carbon nanotubes.

Interfacing Natural and Artificial Membrane Channels with Ion Selective Bioelectronics

Authors: Marco Rolandi, Heather Knight, George Luka

Affiliation: Electrical and Computer Engineering, University of California, Santa Cruz

Abstract: Biological membrane channels enable communication between cells and support molecular recognition. While designing membrane channels from scratch for precise sensing is difficult, an even greater challenge is connecting them to electronic devices for efficient signal readout. An efficient interface for membrane channels will enable new bioelectronic technologies. Here, we create programmable and modular artificial ion-channel interfaces by integrating natural and synthetic membrane pores with cation- and anion-selective contacts. We will present examples including gramicidin, rhodopsins, and DNA nanopores paired with proton-conducting electrodes, as well as chloride channels interfaced with chloride-conducting contacts. We will also discuss potential computing strategies enabled by this platform.

Stacked 2D Materials for Temporal Gating of Ion Transport through Nanopores with both DC and AC Gate Voltages

Authors: Matthew Schiel, Ethan Cao, Aaron Barajas-Aguilar, Javier Sanchez-Yamagishi, Zuzanna Siwy

Affiliation: University of California, Irvine

Abstract: Transport properties of nanopores can be controlled by chemical modification, electrolyte conditions, or placing a gate near or in the pore. Most systems operate with the classical Debye layer such that the changes are slow and allow a electrical double-layer (EDL) to form. Here, we present a nanopore system with 2D gates whose electrical potential is gated by applying DC, AC, or AC with DC offset voltages. We drilled single sub-10nm nanopores by TEM in stacked 2D materials (hBN and graphene) positioned over a 3 μ m diameter micropore in the center of a silicon nitride membrane on a silicon chip. We have tested hBN-graphene-hBN stacks, where a \sim 3nm conducting layer of graphene is encapsulated in between two insulating hBN flakes. We were then able to measure ionic current through the pores with varying KCl concentration using a PDMS conductivity cell. The nanopores exhibit a low concentration conductance saturation indicative of surface charge. We also developed a thin printed circuit board (PCB) to go in our PDMS conductivity cell with coaxial connections to apply high frequency voltages to the chip, and added metal electrodes to the chip with fine metal contacts to the graphene layer of an hBN-graphene-hBN stack. Finally, we deposit SiO₂ layer over the chip, except for a small exposed area over the 2D material, which insulates the electrodes from the fluid. With this we are able to apply both DC and AC voltages to the electrodes on the chip, allowing us to test non- equilibrium EDL gating.

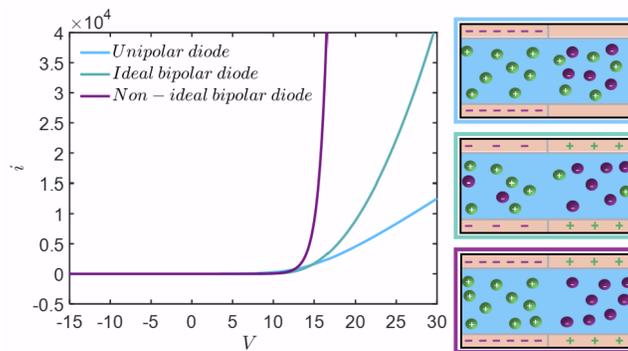
Towards a Unified Understanding of the Electrical Response of Bipolar Nanofluidic Systems

Authors: Ayelet Ben-Kish Sharvit, Yoav Green

Affiliation: Mechanical Engineering Department, Ben-Gurion University, Israel

Abstract: Bipolar nanofluidic systems are used in various applications, including water desalination, energy harvesting, bio-sensing, and fluid-based electrical circuits. Their ability to undertake such a wide range of processes originates at the nanoscale, wherein the electrical charge of the surfaces yields a filter-like property, commonly known as ion selectivity. The selectivity depends on various parameters, such as the surface charge density, geometry, bulk electrolyte concentration, and more. However, to date, no single known theory accounts for all parameters. In fact, several existing models differ in their underlying assumptions on the relative importance of the controlling parameters¹⁻⁴, resulting in different theoretical predictions. In particular, that of the current-voltage response.

In my talk, I will review all three models and their underlying assumptions on the key parameters that control the overall response. Then, using numerical simulations, I will demonstrate when the assumptions break down and why. The understanding gleaned from this work can be used to improve the design of bipolar nanochannels in applications such as water–energy harvesting systems and to improve the interpretation of experimental measurements.



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Nanopores with Dynamic Pore Opening Diameter

Authors: Savannah Silva¹, Anthony Cho¹, Ethan Cao¹, Ivan Vlassiouk², Zuzanna S. Siwy¹

Affiliation: ¹University of California, Irvine; ²Oak Ridge National Laboratory

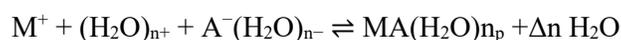
Abstract: Solid state nanopores have emerged as model systems for understanding nanoscale transport properties and serve as templates for designing biological sensors. Unlike their biological inspirations, the majority of nanopores prepared so far have been structurally static devices. If we could prepare nanopores whose opening diameter fluctuated in time with precise control at known locations in the pore, we could create ionic memristors and achieve new transport modes. Here we present ~5nm in diameter single nanopores drilled through a 10nm thick gold layer positioned atop a 30nm thick SiN film. Two types of devices were prepared; one containing single stranded DNA and the other containing hairpin DNA attached to the discrete layer of gold using thiol chemistry. When an external electric field was applied across a nanopore with single stranded DNA, the nanoconfined DNA molecules exhibited steric and electrical constraints that led to memristor-like behaviour in the current-voltage curves. The degree of hysteresis was controlled by salt concentration, voltage and pore diameter. In contrast, nanopores containing DNA hairpins conducted similar currents in forward and reverse bias in agreement with the rigidity of the hairpin molecule. A prototype of a sandwich structure with a 10nm gold layer positioned between 30nm thick SiN and 15nm thick silica layers was fabricated and larger pores of few tens of nm were drilled using focused ion beam. In a three-electrode set-up, an oscillating voltage applied to the gate introduces an additional control of the conformation of the attached DNA and subsequently, the pore diameter. The nanopores presented here present the first steps towards preparation of non-equilibrium nanopore systems.

Ion Pairing in Osmotically-Stressed Environment: Disentangling the Effects of Ion-Ion and Ion-Water Interactions

Authors: Jay Prakash Singh, V. Freger

Affiliation: Technion – Israel Institute of Technology, Haifa 3200003, Israel

Abstract: Efficient ion and salt separations are central to modern technologies, yet transport and thermodynamics in confined and osmotically and mechanically stressed environments, such as polymers and nanomaterials, remain poorly understood. One key challenge lies in computing ion activity, which classical mean-field models (Donnan, Poisson–Boltzmann, Debye–Hückel) treat assuming full dissociation and weak ion-ion interactions. However, they break down in above systems, for which Bjerrum’s ion-pairing concept offers a sounder approach. The distinct feature of ion-pairs is that their formation is influenced not only by ion-ion interaction but also by hydration as well. Thus pairs are qualitatively differentiated as double solvent-separated (2SIP), single solvent-separated (SIP), and contact ion-pairs (CIP), differing the number of water molecules Δn shed upon pairing, expressed as



As water actively participates in this “reaction”, water activity (a_w) strongly modulates the effective association constant K and may enhance under osmotic and mechanical stress enhance pairing. This effect is often overlooked, commonly assuming $a_w \sim 1$ and focusing on ion-ion interactions only. To clarify and quantify significance of hydration, we undertake thermodynamic analysis of pairing in salt solutions under varying osmotic pressure. It rigorously separates variation of K to terms contributed by ion–ion and ion–solvent interactions. We then use molecular dynamics simulations to quantify and compare each term and estimate Δn for several monovalent salts. This quantity determines how water shedding amplifies pairing in confined and osmo/mechanically stressed system, e.g., nanochannels or polymeric membranes, offering insights directly relevant to the modeling and design of ion-selective membranes and nanomaterials.

Keywords: Ion pairing; Electrolyte solution; Molecular dynamics simulations.

Memory in Conical Nanopores Regulated by Electrolyte Composition and Pore Size

Authors: Shiwei Tang, Isaac Hernandez, Anthony Dougman Cho, Claudia Evodie Puspa Dewi, Zuzanna S Siwy

Affiliation: University of California, Irvine

Abstract: Ion dynamics in nanopores offer pathways for unconventional computing, mimicking neural-like oscillations and memory. In this study, we examined how dynamic and reversible precipitation of two types of weakly-soluble salts in single conical nanopores produces a wide range of memory effects. Low concentrations of CaCl_2 or CoCl_2 combined with phosphate buffer were symmetrically applied to conical nanopores. Due to local ion enhancement near the nanopore tip, transient nanoprecipitation of CoHPO_4 and CaHPO_4 results in oscillations or fluctuations in the transmembrane current. In nanopores with an opening diameter below ~ 8 nm, CoHPO_4 produced highly reproducible oscillatory responses, while CaHPO_4 resulted in more fluctuating and less distinguishable current patterns, suggesting a less stable modulation of ionic transport. Ionic memory was largely found in variations in the oscillation pattern dependent on voltage scan direction. Larger nanopores with opening diameter between 9 and 20 nm also produced ion current instabilities when CoHPO_4 and CaHPO_4 were formed in the pore, however, the current switching was more stochastic and occurred at higher voltages compared to sub-8 nm nanopores. Ionic memory in larger pores did not rely on the current instabilities but rather on negative incremental resistance and directionally dependent average current. These observations suggest that both ionic species and pore diameter play a significant role in shaping memory behavior. These findings underscore the importance of electrolyte composition and pore diameter in controlling nanopore-based ionic memory and may provide a basis for engineering more complex iontronic systems through tailored electrolyte selection.

Predicting Adsorption Length Scales in Nanoconfined Fluids: Applications to Generalized van der Waals Confined Equations of State

Authors: Jarrett S. Turner, Sanjay Garimella, Michael S. Strano

Affiliation: Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

Abstract: Nanoconfined fluids exhibit thermodynamics that cannot be described via conventional, bulk equations of state. However, such confined thermodynamic models are essential for understanding nanofluidics and steric-based separations. Current confined equations of state rely on empirically fitted pore-wall interaction parameters. A theory-based framework is proposed to predict the characteristic length scales of adsorption (σ and λ) which constitute the essential length scales underpinning the confined van der Waals and Peng—Robinson equations of state. Closed form approximations for the locations of adsorption layers are derived for slit and cylindrical pores from Lennard-Jones interaction potentials. From these layers, adsorption well-widths and repulsive regions are determined, which are consistent with trends observed in molecular simulations. When incorporated into confined equations of state, the predicted parameters reproduce densities and isobars, with excellent agreement to experimental data for water in carbon nanotubes. The proposed approach offers a closed form method to link microscopic Lennard-Jones interactions to macroscopic thermodynamic equations of state, advancing their predictive capabilities for adsorption, nanofluidics, and separations.

Ion Transport through Single-crystal MOF Membranes

Authors: Camille Violet, Madeleine Gaidimas, Akash Ball, Junwei Zhang, Heather Kulik, Zuzanna Siwy, Menachem Elimelech

Affiliation: Research performed at Yale University, USA; currently work at Lawrence Livermore National Laboratory

Abstract: Developing design principles for next-generation membranes hinges on our ability to relate material characteristics and solute transport behavior. Nanoporous crystalline materials, such as metal-organic frameworks (MOFs) and covalent-organic frameworks (COFs), are ideal models of study because their structure is known with angstrom-scale precision from crystalline unit cells, and their pore chemistry is highly customizable for ion-selective interactions. Prior reports of MOF membranes show promising ion separation capabilities, however these polycrystalline systems with inter-grain transport pathways preclude the ability to directly relate intrinsic MOF properties and transport behavior. In this talk, we present the first single-crystal MOF membrane platform and show that potassium chloride transport through the MOF is highly sensitive to pore chemistry. Ion transport is measured through single crystals of the zirconium-based MOFs: UiO-66-H, UiO-66-NH₂, and UiO-66 NH₃⁺, revealing stark differences between reported polycrystalline MOF membranes and intrinsic MOF properties. This talk raises the question of whether polycrystalline material platforms can effectively harness the active material properties and highlights the importance of well-controlled platforms for mechanistic insight.

Scalable and Tunable Carbon Nanomembranes for Selective Molecular Transport

Authors: Zhen Yao¹, Jan Biedinger¹, Nikolaus Meyerbröker², Martin Wortmann¹, Yang Yang¹, Andreas Hütten¹, Günter Reiss¹, Armin Götzhäuser¹

Affiliation: ¹Bielefeld University, Bielefeld, Germany; ²CNM Technologies GmbH, Bielefeld, Germany

Abstract: Carbon nanomembranes (CNMs), molecularly thin two-dimensional materials with intrinsic sub-nanometer pores, provide a versatile platform for nanofluidics. Their ultrathin structure enables fast molecular flux, while surface chemistry and pore architecture can be tailored for selective transport.

We present a scalable synthesis route based on electron-induced crosslinking of spin-coated poly(4-vinylbiphenyl) films [1], combined with atomic layer deposition (ALD) for pore and surface functionalization [2]. This strategy enables precise tuning of pore dimensions and hydrophilicity, yielding CNMs with water vapor permeance as high as $1.9 \times 10^{-5} \text{ mol s}^{-1} \text{ m}^{-2} \text{ Pa}^{-1}$ and $\text{H}_2\text{O}/\text{N}_2$ selectivity above 10^4 , outperforming state-of-the-art polymer and graphene oxide membranes. These results establish CNMs as promising candidates for energy-efficient dehumidification and gas separation.

Together, these studies demonstrate how scalable fabrication and nanoscale interface engineering translate into tunable nanofluidic transport, highlighting CNMs as a versatile materials platform for separations, sensing, and controlled molecular flow.

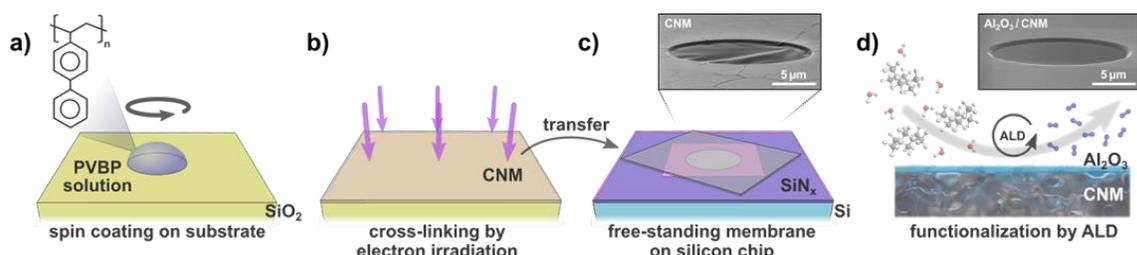


Fig. 1. Steps for the preparation of CNM and subsequent Al_2O_3 functionalization via ALD.

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Two-dimensional Clay Channels for Tunable Nanofluidic Memristor

Authors: Sangeeta Yadav^{1,2,3,†}, Raj Kumar Gogoi^{1,2,†}, Siddhi Vinayak Pandey^{1,2}, Ankit Bhardwaj^{1,2}, Sunando DasGupta⁴, Boya Radha^{1,2,5,*}

Affiliation: ¹Department of Physics and Astronomy, The University of Manchester, Manchester M13 9PL, United Kingdom; ²National Graphene Institute, The University of Manchester, Manchester M13 9PL, United Kingdom; ³Advanced Technology Development Centre, Indian Institute of Technology Kharagpur, Kharagpur 721302, India; ⁴Department of Chemical Engineering, Indian Institute of Technology Kharagpur, Kharagpur 721302, India; ⁵Photon Science Institute, University of Manchester, Manchester M13 9PL, U.K.

Abstract: The dynamic reconfiguration of charge carriers within confined ion channels under electrical stimulation leads to memory effects, wherein the internal resistance state is modulated by the history of the applied electric field. The memory effect exhibited by vermiculite (VM) nanofluidic devices can be harnessed for information storage and processing using a single nanofluidic component. Herein, we report the switching between different memory loop types by tuning ion transport pathways through the channels. The asymmetrical architecture, combined with the intrinsic surface charge of the VM channels, enables voltage polarity-dependent memory switching behaviour: from crossing-1 to crossing-2 loops, and *vice versa*. Furthermore, we demonstrate the evolution of hysteresis properties and rectification across varying voltages, frequencies, and ionic concentrations. The inherent memristive nature of the VM channels is demonstrated using different *in-plane* and *out-of-plane* channel configurations, prepared *via* re-stacked VM membranes and ultramicrotomy, with channel length scales ranging from nanometer to micrometer to centimeter. The VM device also demonstrates essential neuromorphic functionalities, such as, synaptic potentiation-depression and memory retention with programmable retention time scales. The reversible and programmable memory nature of our vermiculite memristors can be optimised based on the application specific use such as cache-like operations and real-time signal processing using STM states or artificial neural networks using LTM states by merely changing the crossing-type. Thus, our memory device offers a cost-effective, scalable fabrication process using natural materials, paving the way for next-generation bio-inspired computing systems.

Direct Imaging Reveals Electromechanical Blistering-based Ionic Memory in Two-Dimensional Nanochannels

Authors: Kalluvadi Veetil Saurav^{1,2*}, Nathan Ronceray^{3,9*}, Baptiste Coquinot⁴, Agustin D. Pizarro³, Ashok Keerthi^{1,2,6}, Theo Emmerich^{3,5,#}, Aleksandra Radenovic^{3,7,#}, Boya Radha^{2,6,8,#}

Affiliation: ¹Department of Chemistry, School of Natural Sciences, The University of Manchester, Manchester, U.K.; ²National Graphene Institute, The University of Manchester, Manchester, U.K.; ³Institute of Bioengineering, School of Engineering, EPFL, Lausanne, Switzerland; ⁴Institute of Science and Technology Austria, Austria; ⁵Laboratoire de Physique, UMR CNRS 5672, ENS de Lyon, Université de Lyon, Lyon, France; ⁶Photon Science Institute, The University of Manchester, Manchester, U.K.; ⁷NCCR Bio-Inspired Materials, EPFL, Lausanne, Switzerland; ⁸Department of Physics and Astronomy, School of Natural Sciences, The University of Manchester, Manchester, M13 9PL, U.K.

Abstract: Nanofluidics, the study of fluid behaviour at the nanoscale, has developed over the past two decades as a transformative yet relatively underexplored field¹. Central to nanofluidics is the non-linear ion transport, where ion behaviour diverges from classical predictions due to extreme confinement, surface effects, and electrostatic interactions within nanochannels². These complexities make the field a “blind spot” for predictive modelling, and traditional continuum theories often struggle to accurately depict the complex coupling between nanoconfined ion dynamics, interfacial forces, and mechanical deformations, necessitating advanced theoretical and computational approaches that incorporate device dynamics.

Nanofluidic memristors are an exciting development in this field, forming the foundation for neuromorphic computing^{3,4}. However, their working principles have been mainly inferred from current–voltage characteristics and theoretical models. By combining electrokinetic measurements with real-time optical thin-film interferometry⁵, we show that the hysteresis responsible for memristive behaviour stems from voltage-induced nanoscale blisters in the confining walls. Additionally, we observe both unidirectional and bidirectional responses, caused by different mechanisms such as electrostatic screening of surface charges and osmotic pressure generated by concentration polarisation. Beyond memristors, this correlational approach provides a powerful means to investigate and control molecular transport at the nanoscale, with wide implications across energy, sensing, and computing.

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