Membrane Society of Australasia



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IMSTEC2025 Q&A





The Membrane Society of Australia (MSA) recently interviewed Associate Professors Amir Razmjou and Jingwei Hou, chairs of IMSTEC 2025, to discuss the significance of this flagship conference, emerging trends in membrane technology, and opportunities for researchers and industry professionals. To be held on the Gold Coast, Queensland, in December 2025, IMSTEC 2025 promises to be a pivotal event for the global membrane community. We have included the key questions and responses from the interview, offering insights into the conference's impact and the future of membrane science.

1. What makes IMSTEC 2025 special, and what broader impact do you hope it will have on the future of membrane technology?

Response: Associate Professor Amir Razmjou emphasised that IMSTEC 2025 is a flagship event for the MSA, marking one of the first major in-person gatherings post-COVID. It offers a unique platform for early-career researchers (ECRs) to network with senior scientists and industry experts, fostering mentorship and collaboration. The conference will showcase advancements in membrane applications, from traditional desalination to emerging fields like mineral processing and biomedical uses, driving sustainability and innovation. Associate Professor Jingwei Hou highlighted the conference's 20-year legacy, noting its role in connecting Australian researchers with global leaders. He envisions IMSTEC 2025 as a catalyst for translating fundamental research into practical solutions, addressing global challenges in water treatment, resource recovery, and beyond.

2. How does IMSTEC 2025 act as a connector across diverse membrane research areas, such as desalination, mineral processing, and biomedical applications?

Response: Associate Professor Amir Razmjou explained that membrane research has evolved significantly over the past decade, shifting from pressure-driven processes like reverse osmosis for desalination to new applications in mineral recovery, selective membranes, and biomedical fields like drug delivery. IMSTEC 2025 will facilitate discussions on these emerging trends, leveraging knowledge from water treatment to accelerate sustainable practices in other industries. Associate Professor Jingwei Hou added that the conference brings together researchers working on fundamental science and those focused on practical applications, creating a critical mass to explore interdisciplinary opportunities and drive innovation across diverse sectors.



3. What emerging trends or innovations in membrane technology are you most excited to see showcased at IMSTEC 2025?

Response: Associate Professor Jingwei Hou expressed excitement about the transition in membrane applications, from water treatment to gas separation, drug delivery, and mineral processing. He highlighted advances in materials like metal-organic frameworks (MOFs) and zeolites, which are opening new possibilities. IMSTEC 2025 will serve as a platform to showcase these innovations, bridging fundamental research with practical technologies. Associate Professor Amir Razmjou echoed this, noting that the conference will highlight how knowledge from mature fields like desalination can be applied to emerging areas, enhancing sustainability and reducing environmental footprints in industries like mining and pharmaceuticals.

4. How does IMSTEC 2025 facilitate the translation of membrane research into realworld applications and connect academia with industry?

Response: Associate Professor Amir Razmjou emphasised that IMSTEC 2025 is a vital bridge between academia and industry, showcasing advanced materials like MOFs and zeolites for new applications. The conference attracts investors and industry partners interested in high-risk, high-reward technologies, fostering collaborations that turn research into scalable solutions for mining, pharmaceuticals, and food processing. Associate Professor Jingwei Hou added that IMSTEC aligns academic research with industry priorities, such as cost and efficiency, enabling researchers to understand real-world needs and work together on impactful solutions.

5. What role does IMSTEC 2025 play in creating opportunities for ECRs?

Response: Associate Professor Amir Razmjou stressed that IMSTEC 2025 is invaluable for ECRs, offering opportunities to build networks, secure mentorship, and gain visibility for funding or industry roles. By connecting with senior researchers and industry professionals, ECRs can learn about publishing in high-impact journals and explore career paths. Associate Professor Jingwei Hou reflected on his own experience as an ECR, noting that conferences like IMSTEC helped him understand the broader research landscape and define his career. He emphasised that IMSTEC 2025 allows ECRs to build a career structure, meet global leaders, and avoid pursuing misaligned research directions.

6. With many global conferences, what are the top three reasons researchers and professionals should attend IMSTEC 2025?

Response: Associate Professor Jingwei Hou outlined three key reasons: (1) IMSTEC's established reputation as a premier platform for membrane science, (2) its role in connecting Australian researchers with global leaders in water treatment, mineral processing, and renewable energy, and (3) Australia's position as a hub for membrane innovation despite its smaller population. Associate Professor Amir Razmjou added that the conference features a diverse lineup of keynote speakers from North America, Europe, the Middle East, and East Asia, offering global perspectives. Held in the stunning Gold Coast in December, it combines scientific excellence with tourism appeal, making it an ideal venue for networking and collaboration.

7. What message would you share with the global membrane community about joining IMSTEC 2025?

Response: Associate Professor Amir Razmjou invited the global membrane community to join IMSTEC 2025, highlighting its role as a hub for building relationships, exchanging ideas, and exploring Australia's innovative membrane research. The Gold Coast's beautiful setting and proximity to East Asia make it accessible and appealing, with opportunities for industry investment in early-stage technologies. Associate Professor Jingwei Hou emphasised Australia's unique position between East and West, facilitating technology transfer and collaboration. He encouraged attendees to engage with local researchers and industry leaders to shape the future of membrane technology.

8. What is your long-term vision for IMSTEC and its role in the membrane community?

Response: Associate Professor Jingwei Hou envisions IMSTEC as an iconic event for the global membrane community, fostering engagement with local and international researchers. He hopes to expand its reach, potentially to New Zealand, while maintaining its focus on collaboration and innovation. Associate Professor Amir Razmjou sees IMSTEC accelerating the industrial adoption of membrane technologies in new sectors like pharmaceuticals and agriculture, increasing industry participation to drive sustainable solutions and cementing the conference's role as a catalyst for innovation.

Quantum Electrons to Next-Gen Membranes: How DFT and MD are Reshaping Separation Science?



BY JAVAD FARAHBAKHSH, MEHDI KHIADANI

Opening Hook

In 1964, three physicists—Pierre Hohenberg, Walter Kohn, and Lu Sham—revolutionised our understanding of matter with the birth of density functional theory (DFT). Originally developed to simplify the quantum manyelectron problem, DFT has since become a cornerstone of modern materials design for chemists, with the efforts of John Pople, which was then led to the Nobel Prize for Pople and Kohn in 1998 (<u>Nature materials</u>).



The Quantum Leap: DFT Enters Membrane Science

DFT began with a simple but profound idea that the electron density of a system holds all the information needed to predict its properties. For decades, this theory was used to study crystals and metals. But by the 1990s, as computing power surged and better exchange-correlation approximations emerged, DFT started venturing into "messier" systems like soft matter and biomembranes.

One of the first breakthroughs came in biological ion channels. Researchers used DFT to model how ions like K⁺ or Na⁺ pass through narrow, selective pores such as the KcsA potassium channel or gramicidin A. These studies revealed critical quantum effects such as polarization and electron density redistribution offering insights beyond what classical models could predict (<u>Biochimica et Biophysica Acta</u>).

Engineering Materials on Fabricated Membranes via DFT

The 2010s marked DFT's transition from biology to membranes, particularly those made from advanced nanomaterials. The application of DFT to these materials opened a new avenue for research within the membrane community.



Graphene Membranes: DFT study showed that angstrom-sized pores in functionalized graphene could separate gases like H_2 and CH_4 with theoretical selectivity up to 10^{23} , far beyond polymer membranes (<u>Nano Letters</u>).

MOF-based Membranes: DFT simulations opened a new frontier in gas separation by screening over 1,200 MOFs for CH_4/H_2 selectivity. The study revealed that materials with pore sizes just large enough to fit a single CH_4 molecule offered superior separation performance (<u>Chemical</u> <u>Engineering Science</u>).

Beyond the Limits: Quantum Computing Meets DFT

Despite its success, DFT faces computational limitations, with its cost scaling cubically as the system size grows (<u>Quantum physics</u>). For membranes involving thousands of atoms, especially with interfaces and defects, full DFT calculations become impractical.

This is where quantum computing enters the scene. Algorithms like the variational quantum eigensolver (VQE) aim to solve parts of the Schrödinger equation on quantum hardware, offering potential proposals speedups. Early suggest combining classical DFT with quantum accuracy subroutines to improve or scalability (SciPost Physics).

The Molecular Motion Picture: MD Brings Dynamics to Membranes

While DFT gives us the "snapshots" of quantum interactions, molecular dynamics (MD) simulates the "movie", in fact, the motion of atoms and molecules over time.

• Water Desalination: In 2012, Cohen-Tanugi and Grossman used MD to simulate water and ion flow through graphene nanopores. Their study showed that water could pass through pores efficiently while salt was blocked—predicting permeabilities orders of magnitude higher than traditional RO membranes (<u>Nano letters</u>).

• **Nanopore Transport:** MD uncovered that water moves through carbon nanotubes in near-frictionless chains, helping explain the high flux in nanochannel membranes.

• Interfacial Behaviour: MD simulations also revealed how membranes interact with solutes, foulants, and solvents which is critical for understanding real-world challenges like fouling or responsive behaviour in "smart" membranes.

Today, MD allows scientists to observe membrane behaviour over microsecond timescales, capturing atomic-level details of polymer motion, ion accumulation, and dynamic pore transformations.

Where We're Heading: Synergy and Scale

The most exciting development is the synergy between DFT and MD. With DFT, we now design materials down to the electron level; with MD, we track how these materials behave in action. In the future, multi-scale simulations will combine the strengths of both, linking quantum accuracy to real-time dynamics across entire membrane modules.

With computing quantum emerging, membrane science has entered a new era, where modelling electrons, atoms, and flow patterns becomes seamless. Coupled with experimental innovations and the discovery of advanced materials through new chemistries, this progress promises faster, affordable, and more more selective membrane technologies. The future of membrane science looks promising as modification advanced surface and quantum computing continue to progress, offering novel pathways to design nextgeneration membranes, ultimately transforming global strategies for water purification, energy generation, and broader sustainability efforts.

Multiscale Modeling in Membrane Science - This comprehensive diagram illustrates the hierarchical relationship between computational modeling approaches across twelve orders of magnitude in both temporal (10⁻¹² to 10⁵ seconds) and spatial scales $(10^{-10} \text{ to } 1 \text{ meter}).$



At the quantum scale, ab-initio calculations and electronic structure methods operate within picosecond timeframes (10⁻¹² seconds) for systems containing tens to hundreds of atoms (10⁻¹⁰ to 10⁻⁹ meters), enabling the investigation of gas-membrane interactions, adsorption energies, and selectivity mechanisms at the molecular level in materials such as zeolites, metal-organic frameworks, and polymer membranes.

Molecular dynamics (MD) simulations span the picosecond to microsecond regimes $(10^{-12} \text{ to } 10^{-6} \text{ seconds})$ while handling systems of 10³ to 10⁶ atoms across nanometer length scales (10⁻⁹ to 10⁻⁷ meters), facilitating the study of permeant diffusion pathways, membrane swelling, and polymer chain dynamics in selective barriers, with accelerated MD and kinetic Monte Carlo methods extending temporal accessibility to milliseconds (10-3 seconds) to capture rare permeation events and long-term membrane stability.

The mesoscale transition occurs around 10⁻⁶ to 10⁻⁴ meters, where atomistic modeling incorporating dislocation dynamics operates on millisecond to second timescales (10⁻³ to 1 second) for systems containing millions of atoms, allowing investigation of membrane morphology, pore formation, and mechanical properties under operating conditions.

At the continuum level, thermo-chemical models and finite element simulations dominate the range from micrometers to meters (10⁻⁶ to 1 meter) over timescales extending from seconds to days (1 to 10⁵ seconds), enabling analysis of membrane modules, concentration polarisation, fouling dynamics, and full-scale separation processes where membrane performance is evaluated under realistic industrial operating conditions with feed pressures, temperature gradients, and multi-component mixtures.

MSA Spotlight Interview: A/Prof. Qiang Fu

EDITED BY HOSEONG HAN, MILTON CHAI



Top: A/Prof. Qiang Fu; Bottom: Dr. Hoseong Han

Hoseong: Hi, A/Prof. Qiang Fu. Thank you very much for joining our MSA Spotlight interview today!

Qiang: Hi! Nice to meet you, and thank you for having me. It's a pleasure to be here.

Hoseong: Shall we dive into the first question? Could you tell us about your research journey and how you got into membrane science?

Qiang: Absolutely! I began with a background chemical engineering and polymer in science. During my PhD, I focused on synthesising various types of polymers using techniques like RAFT and ATRP. Even then, I kept wondering: how can these complex polymers be applied in real-world scenarios? That curiosity led me to join Professor Greg Qiao's group, where we worked on nanoengineering polymer membranes for CO₂ separation. This is an area relevant to climate change, which made the work even more meaningful. Over time, we transitioned from high-performance lab-scale membranes to practical thin selective layers supported by robust mechanical substrates, significantly improving permeance and selectivity.

Hoseong: That's a fascinating start! How did your PhD and postdoc experiences shape your current direction?

Qiang: They laid a strong foundation for my career. My PhD focused on polymer chemistry, while my postdoc work was rooted in chemical engineering. This combination helped me cultivate both scientific curiosity and a practical, solution-oriented mindset. It's been particularly helpful in my current work on interfacial solar evaporation (ISE), where understanding both molecular-level interactions and system-level engineering is essential.

Hoseong: What is your current research focus?

Qiang: Since joining UTS in 2019 with a fellowship, I've focused on water treatment, particularly interfacial solar evaporation (ISE). It might sound simple, just using sunlight to evaporate water, but it's surprisingly complex and rich in scientific challenges. Traditional solar distillation systems yield around 0.5 kg of water per m² per hour.

Qiang: By incorporating polymer-based hydrogels and photothermal materials, we've pushed this up to 3.5 kg/m²/h, well beyond theoretical limits. Now, we're working to understand the fundamental mechanisms behind this and scale the technology for real-world applications such as desalination and water purification.

Hoseong: That's incredibly impressive. Could you explain the mechanism your team is exploring in these evaporation membranes?

Qiang: We're systematically testing different hydrogels with varying functional groups. Interestingly, we've observed that relatively neutral, hydrophilic groups, such as those found in polyacrylamide or poly(ethylene glycol), tend to promote evaporation. So, it's not just about incorporating photothermal materials. The key lies in the subtle molecular interactions between water and polymer background networks. My in polymer chemistry has been particularly valuable in this area. While we haven't pinpointed a definitive mechanism yet, we're actively optimising and conducting further studies to gain deeper insights.

Hoseong: Are there interdisciplinary aspects in your current work?

Qiang: Absolutely. We collaborate with simulation experts to model how water molecules interact with polymer matrices, and with fluid dynamics researchers to design systems that efficiently transport and condense vapour. It's a highly collaborative field, and integrating knowledge from multiple disciplines is essential to developing functional, scalable ISE systems.

Hoseong: What trends or challenges do you see in membrane science?

Qiang: I see growing interest in combining separation processes with directional mass transfer.



Qiang: For example, leveraging sunlight and evaporation not just to purify water, but also for selective ion separation or even energy generation. It's about making membranes to do more by harnessing directional thermal and mass transport phenomena.

Hoseong: For the next question, I'd like to talk a bit more into your career path. What were some turning points along the way?

Qiang: Securing fellowships was definitely pivotal. Early in my career, I was mostly involved in industry-funded research, which limited my flexibility. Receiving the ARC Super Science Fellowship gave me the time and stability to pursue fundamental ideas. Later, the Future Fellowship allowed me to supervise PhD students, manage funding, and truly grow as an independent researcher. **Hoseong:** Who were your key mentors and collaborators?

Qiang: I've been fortunate to work with some incredibly supportive mentors. Prof. Qiao taught me how to lead a research group and motivate students effectively. Prof. Webley and Kentish were incredibly generous with their time and consistently supported students' development. While Prof Nghiem and Shon provided critical support after I transitioned to UTS. Each mentor and collaborator has brought something unique, and I've made it a point to learn as much as possible from all of them.

Hoseong: What achievements are you most proud of so far?

Qiang: In addition to the fellowships, I'm especially proud of having three cover articles, two on gas separation and one on solar evaporation. Seeing our research highlighted that way, including the visual design, was incredibly rewarding. I even have them framed in my office!

Hoseong: As an early-to-mid-career researcher, what challenges have you faced during the transition?

Qiang: Honestly, the biggest challenges are definitely human resources and funding. They're two sides of the same coin. More students and funding lead to more progress and publications, but breaking into that cycle can be tough. Also, scaling up lab-based discoveries for industrial applications remains a tough hurdle due to the gap between fundamental research and industrial demands.

Hoseong: How do you engage with industry as an early-career researcher?

Qiang: listening, really lt starts by understanding problems industry the partners are facing. Once you do that, collaboration becomes more natural. For early- and mid-career researchers like me, partnering with senior colleagues can be very especially when it comes helpful, to technology scale-up. And I'd say, don't be afraid to ask for help, most senior researchers are more than willing to support you.

Hoseong: With so much going on, how do you balance your research with teaching and administrative responsibilities?

Qiang: Honestly? (chuckles) You just have to work hard. There's no magic formula. I typically spend 2 to 3 days preparing and delivering lectures, answering student questions, and managing responsibilities. It's demanding, but teaching also builds essential academic skills that pay off in the long run.

Hoseong: Thank you so much for sharing your journey with us. It's been a really insightful conversation. From polymers to practical uses, your story shows how deep science and real-world impact can go hand in hand. Looking forward to seeing where your work takes you next!

Qiang: Thank you very much for the kind words! It's been a real pleasure to have this conversation. I hope we cross paths again soon!

Scientific Interview: Prof. Mehdi Khiadani

EDITED BY YASAMIN HAMIDIAN, JAVAD FARAHBAKHSH

In this academic engagement section, we had an interview with Prof. Mehdi Khiadani from Edith Cowan University (ECU). Prof. Khiadani is a Professor in the School of Engineering and has been instrumental in transforming ECU's engineering research fluid landscape. His journey from mechanics membrane technology to represents a fascinating evolution of research interests leadership and excellence.



Top: Prof. Mehdi Khiadani; Bottom: A/Prof. Amir Razmjou

Amir: Thank you for joining us today for the MSA newsletter interview. Could you walk us through your educational and professional journey chronologically, starting from your bachelor's degree?

Mehdi: Thank you, Amir. I completed my bachelor's degree in water engineering in Iran in 1988. Then, I moved to Australia where I had admissions from both University of Wollongong and UNSW. **Mehdi:** I chose UNSW to pursue my master's degree in water engineering at the School of Civil and Environmental Engineering, which I completed around 1994. After a gap period that I spent for searching suitable PhD opportunities, I was drawn to the University of Technology Sydney (UTS), where experimental work was underway to revise the Australian standards for roof drainage gutters. I found this a very exciting project and I applied for that.

Mehdi: Well, I have to say that I was fascinated by the interaction between the incoming flow and the gutter flow, an area that posed significant challenges and had virtually no existing research at the time. This curiosity became the turning point of my academic journey, leading me to commence my PhD at UTS in late 1995. Since UTS did not have the required laser Doppler measurement equipment, I conducted my experimental work at the University of Wollongong, through a collaboration facilitated by Professor Simon Beecham. I successfully completed my PhD in early 2000.

Amir: What happened after your PhD completion?

Mehdi: I spent three years working in consulting roles with prominent engineering companies beginning with WSP, followed by Aurecon, and then AECOM. These were excellent opportunities that allowed me to grow rapidly in the water engineering industry.

However, I was always fascinated by teaching and research. During one year of industry work, I actually split my time between parttime industry work and part-time postdoctoral research at UTS. Eventually, I returned to Iran where I worked as an academic for seven years, gaining exposure to environmental engineering and healthrelated applications.

Amir: How did you transition to ECU?

Mehdi: Well, I found a very interesting position at ECU in 2011, and following a successful interview, I commenced as a Senior Lecturer in April of that year. Just three months later, I was appointed as the Higher Degrees Coordinator at a time when ECU was expanding its School of Engineering. When I began, there were fewer than 10 research students, with many taking between 5 to 7 years to complete their degrees. **Mehdi:** Then, I undertook a comprehensive refurbishment of the HDR program and began actively recruiting PhD students. In 2016, I was appointed Associate Dean (Research), a role I held for six years until the end of 2021. By the time I stepped down, the School had grown to approximately 90 full-time PhD students.

Amir: Can you tell us about your academic promotions?

Mehdi: I was recruited as Senior Lecturer in 2011, promoted to Associate Professor in 2016 when I became Associate Dean Research, and achieved full Professor (Level E) in 2024. My journey has been a combination of teaching, research and leadership roles, which was very rewarding as I helped establish and expand ECU's engineering school.

Amir: When did you first encounter membrane technology?

Mehdi: Well, that is a very interesting question. I should say my initial exposure to membrane technology dates back to 2017. I had a PhD student who wanted to use renewable energy for water treatment and desalination. Before that, we were working on thermal-based desalination using flash evaporation systems.

In late 2016 or early 2017, I was introduced to membrane distillation. We purchased hollow fiber membranes and coupled them with renewable energy heat pipes.

Because of my background in civil engineering, I focused my research on integrating membrane distillation with renewable energy sources and low-grade waste heat.

Amir: Why did you choose this processfocused approach rather than material development? Mehdi: I was always intrigued by the sight of solar panels on rooftops and envisioned that, one day, other systems could also be installed to harness solar energy for water treatment. This concept is particularly relevant for managing household wastewater in urban settings, as well as addressing water scarcity in remote communities that often lack reliable access to clean water. It also holds promise for desalinating bore water, treating saline water, and supporting coastal communities. I saw this as a field where I could make a meaningful and lasting contribution.

Amir: How has your industry engagement evolved, particularly regarding membrane technologies?

Mehdi: My industry engagement started seriously in 2018, primarily through collaborations with Water Corporation in Western Australia on wastewater and water treatment projects. Initially, these projects had limited focus on membrane technologies. However, after you joined ECU, new opportunities emerged to explore a broader range of membrane types. Your expertise in this field has been instrumental in expanding our membrane-related industry collaborations and securing more targeted research projects in this area.

Amir: What advice would you give to early career researchers wanting to transition to stable academic careers?

Mehdi: From my leadership experience working with industry, I have learned two critical lessons. First, Australian industry generally seeks ready-made, off-the-shelf solutions. Second, a communication gap often exists between academia and industry. Manv researchers approach industrv interactions with an academic mindset usually focusing on publications and research outcomes, while industry stakeholders are more interested in how we can help improve their operations, increase profits, and reduce costs.

Mehdi: I believe it is essential for researchers to learn the language and expectations of industry. I strongly recommend pursuing industry-focused training, seeking mentorship from experienced industry collaborators, and observing successful academics who have built strong industry partnerships. Start by engaging with smaller funding opportunities and gradually work towards larger projects. It's important to recognize that industry typically turns to academia only when they encounter challenges they cannot resolve internally.

Amir: Where do you see the future of membrane technology research?

Mehdi: While membrane technology for water and wastewater treatment is wellestablished, significant opportunities remain, particularly in addressing persistent operational challenges faced by industry. One critical issue is membrane lifecycle management. After several years of use, membranes must be either disposed of in landfills or recycled, which can definitely raise sustainability concerns. I believe membrane recycling is increasingly important, as water authorities accumulate large volumes of spent membranes requiring responsible disposal. desalination With expanding globally, this can potentially become a major issue.

Other important areas could be circular economy applications, selective resource recovery in mining, and selective ion separation for valuable materials like lithium. I have to emphasise that fouling still is and need challenging we better understanding of how variable renewable energy affects membrane performance, such as how variable speed pumps impact fouling. Energy optimisation is also critical for making membrane technologies more sustainable and cost-effective.

Amir: Coffee or tea?

Mehdi: Coffee! I was a tea person before joining ECU, but my attitude changed, and I switched to coffee. Coffee is my first choice these days.

Amir: If you could choose a different profession, what would it be?

Mehdi: I'd still be a water engineer. I'd still choose engineering because water engineering helps with health and food security. Many people still struggle with water access. I can't think of any other area. I don't regret my choice.

Amir: If you had to choose one city to spend the rest of your life, which would it be?

Mehdi: Perth is the best! Before coming to Perth, I thought it was the most isolated place in the world, but you need to live in Perth to understand it. Before joining Perth, I had a different impression. Now I have another impression – it's my city now.

MSA Spotlight Interview: Rokhsare Kardani

EDITED BY HOSEONG HAN, MILTON CHAI



Top: Rokhsare Kardani; Bottom: Dr. Hoseong Han

Hoseong: Hi, Rokhsare, thank you so much for taking the time to chat with me! Would you like to start by introducing yourself?

Rokhsare: Absolutely! My name is Rokhsare, but most people call me Rokhi. I'm currently a PhD student majoring in Environmental Engineering. Before this, I studied Chemical Engineering for my Master's, focusing on membrane separation. That's actually what I continue to work on now. Specifically, using membranes for water and wastewater treatment.

Hoseong: Great! What led you to pursue a PhD, especially in membrane research?

Rokhsare: Well, I've always had a strong concern for the environment, and during my Master's, I began working on membrane fabrication. I found the process of making and improving membranes really satisfying. It just clicked for me. I'm motivated by the desire to do more, and PhD research gives me that opportunity. **Hoseong**: Could you walk us through your current research project?

Rokhsare: My work focuses on removing contaminants like salts and heavy metals from wastewater. I'm using biopolymerbased hydrogels for this. The goal is to improve water quality, and hopefully in the future, I can contribute to the water industry by working on real-world applications of this technology.

Hoseong: That's really exciting. So your work seems to have industry potential. Do you eventually want to move into that space?

Rokhsare: I would love to have multidisciplinary experience, so I'd like to work in industry to better understand how research translates into real-world impact, particularly in roles related to water quality monitoring and treatment. Places like environmental consultancies always need people with this background, so that's where I see myself.



Hoseong: Nice! My next question is, how does your research fit into the broader goals of your lab or university?

Rokhsare: In our group, many of us work with for various water hydrogels treatment applications. While I'm using them as membranes, some of my colleagues are using them as adsorbents. We share our experiences, techniques, and challenges. It's a really collaborative environment, and we help each other improve. At the university level, our work contributes to producing high-quality research and publications, which hopefully the field of environmental advance engineering.

Hoseong: It sounds like a very supportive space. So what's been the most exciting moment of your PhD so far?

Rokhsare: Oh, definitely last year's school showcase!

Rokhsare: I joined the School of Civil and Engineering's Environmental research competition mostly to practice public speaking, but I ended up winning first place! I was shocked and thrilled. There were also people from the industry in the audience, and I think my simple, clear explanation helped them connect with the importance of my work. I also presented at the MSA Annual Meeting and won the Runner-Up award for my poster. These experiences have really boosted my confidence.

Hoseong: Huge congratulations! That's such an achievement, especially in your second year. How about recent publications?

Rokhsare: Yes! I just had a paper published in the Journal of Hazardous Materials. It's a highly regarded journal with a strong impact factor, so I'm really proud of that.

Hoseong: Congratulations again! Now let's talk challenges. What's been one of the toughest moments in your PhD journey?

Rokhsare: Lab work can be really tough. In the second chapter of my thesis, I struggled to fabricate a membrane using a new method. I was suggested simplifying it, but I really wanted to make that method work. So I kept trying and eventually, I succeeded. That experience taught me a lot about persistence and trusting my instincts.

Hoseong: Has your perspective on your research changed since you started?

Rokhsare: Definitely. At the beginning, I had these big, idealistic goals. But working in the lab helps you realise the importance of being realistic, balancing ambition with available resources and time. You start to value progress over perfection.

Hoseong: Totally relatable. What skills or lessons do you think will be most valuable in your future?

Rokhsare: Confidence and experimentation. I've learned to stop overthinking and just try things out. Also, networking has been a big one. A casual lab chat can sometimes solve a problem you've been stuck on for days!

Hoseong: Where do you see your research going in the next few years?

Rokhsare: The field of water treatment is expanding, and there's still so much to explore, new materials, new fabrication techniques, and better testing. I think scalability will be the next big challenge. If we can make these materials work on a larger scale, the impact could be huge.

Hoseong: Do you think you'll stay in academia or move to industry?

Rokhsare: Industry, most likely as I answered earlier. But I'd love to stay connected to the university, maybe collaborate or attend academic events. I like the idea of bridging both worlds.

Hoseong: How do you hope your research will help solve real-world problems?

Rokhsare: Even the smallest steps in research contribute to a larger solution. My current work may be challenging to scale, but every improvement in material stability or performance brings us closer to addressing global water issues. That's what keeps me motivated.

Hoseong: That's inspiring. What advice would you give to incoming PhD students, especially those in membrane science?

Rokhsare: Read widely, experiment often, and attend events. Present your work and connect with people. It makes a huge difference. And most of all, enjoy your time at uni. It's a unique and rewarding experience. **Hoseong**: And what would you say to someone unsure about starting a PhD?

Rokhsare: It depends on the person. If you love studying and being in an academic environment, go for it. It's challenging but fulfilling. But if you're not passionate about research, there's no harm in exploring other paths first, you can always come back later.

Hoseong: Last fun one, if you could solve any scientific problem instantly, what would it be?

Rokhsare: I'd make it possible to convert seawater into high-quality drinking water instantly. Especially for countries like Iran, where water scarcity is a big issue despite being near the sea. That would be amazing.

Hoseong: Amazing! It's been such a pleasure chatting with you. Thanks again for taking the time to share your journey with us!

Rokhsare: No worries at all! Thanks for having me. It was a pleasure!

Enhanced Quantum Capabilities in Membrane Design for Ion Separation Using Machine Learning Models



BY AMIN SARMADI, MEHDI KHIADANI

Ion separation is critical for resource recovery from waste tailings but presents significant challenges. Lithium recovery benefits from its distinct ionic size and hydration energy, whereas separating ions like Ni²⁺ and Co²⁺—which have nearly identical properties and are prevalent in spent batteries (e.g., LiNi_{0.8}Mn_{0.1}Co_{0.1}O₂)—is far more complex. Quantum mechanics, though seems abstract, offers a promising approach by elucidating molecular-level interactions essential for selective ion separation (<u>Kim et al., 2021</u>; <u>Violet et al., 2024</u>).



Figure 1. A database of functional groups is encoded, DFT provides a subset for ion-binding affinities, a neural network predicts affinities, top candidates for suitable functional groups are validated experimentally, and active learning optimises the search (<u>Violet et al., 2024</u>).

The Nature Water paper by Violet et al., led by Professor Menachem Elimelech, provides valuable insights into this field. It highlights how functional groups exhibit preferential affinity for specific ions in the presence of competing ions. The paper explores the guantum mechanical and molecular origins of this selectivity, noting that ion-binding affinity stems from quantum-level interactions. For example, Ni²⁺ and Co²⁺, despite their similar sizes, interact differently with ligands due to quantum effects rooted in molecular orbital theory. These effects govern binding strength and ion specificity, enabling membranes to exploit subtle differences in ionic interactions (Violet et al., <u>2024</u>).

Quantum mechanical calculations, such as Density Functional Theory (DFT), estimate interaction energies between ions and functional groups by solving the electronic structures of these complexes. Hiahthroughput DFT calculations on a subset of molecules from a candidate database can generate a training dataset. This binding affinity data can then train a neural network to create a surrogate model for predicting affinities. Inspired by drug discovery, this approach mirrors virtual high-throughput screening (VHTS), which evaluates billions of compounds daily to identify those with target ion-binding affinities, far surpassing exclusive experimental methods. In drug discovery, vast compound libraries are screened to predict binding affinity to protein receptor sites. Similar screening methods could be extended to identify selective functional groups to accelerate ion-specific membrane design. The goal is to narrow the vast chemical search space to a manageable set of candidates (e.g., 10-100 molecules) for experimental evaluation in ion separation. Active learning further refines this process by identifying the next-best molecule from the database for iterative model improvement (Figure 1) (Violet et al., 2024).

Practical challenges, however, persist. While quantum mechanics provides deep insights, real-world obstacles-such as synthesising materials precise with properties, scaling production, and ensuring industrial compatibility-remain significant. Balancing these with cost and durability limits quantum's immediate applicability. Nevertheless, its ability to reveal ion behavior at the atomic level, combined with machine learning models that efficiently process vast datasets, can be a gamechanger for ion separation, transforming resource recovery into a sustainable reality.

Accelerating Materials Discovery with Machine Learning and Quantum Accuracy



BY HOSEONG HAN, MEHDI KHIADANI

How can we efficiently and accurately access the molecular-level properties of materials?

Traditionally, methods like molecular dynamics (DM) simulations based on density functional theory (DFT) have been used to predict structural and dynamic behaviours with high accuracy. However, simulations are computationally such expensive, often limited to a few hundred atoms and short timescales (picoseconds), making them impractical for studying longtime dynamics or large systems.

In a recent study, Sharma and Sanvito introduced a novel workflow that combines quantum chemistry with machine learning, offering a solution to these limitations. By using a machine learning model called the Spectral Neighbour Analysis Potential (SNAP), trained on carefully selected DFT they achieved quantum-level data, accuracy at a fraction of the computational cost.

What sets their approach apart is the use of a temperature-driven active learning algorithm, which drastically reduces the number of DFT calculations needed. This method efficiently samples diverse atomic environments by gradually increasing simulation temperature, ensuring coverage of a broad range of structural configurations. As a result, the researchers successfully modelled two benchmark metal-organic frameworks (MOFs), ZIF-8 and MOF-5, capturing their vibrational properties, thermal expansion and even internal rotational dynamics with excellent agreement to experimental data.

This development is particularly promising for applications such as membrane-based gas separation, adsorption, and catalysis, where MOFs play a central role. Moreover, the same strategy can be extended to other materials beyond MOFs, streamlining the materials design process by identifying high-potential materials to accelerate advanced materials discovery.

Although the method is still in its early stages, this work highlights the transformative potential of combining chemistry, DFT, and quantum active machine learning. It opens the door to fast, accurate, and scalable materials simulations, ultimately saving time and resources in both academic and industrial research.



DFT reveals electron response in DNA base pairs to laser pulses. (<u>Source</u>)

Industry Engagement Interview: **Dr. Sebastien** Allard

EDITED BY SHAYAN ABRISHAMI, MILTON CHAI

This edition of the Membrane Society of Australasia (MSA) newsletter spotlights Dr. Sebastien Allard, a water chemist at CSIRO driving innovation in membrane technology. From his pioneering work on electrodialysis reversal and bipolar membranes, to solutions for water scarcity and resource recovery, Dr. Allard's expertise is shaping a sustainable future. Dive into his Q&A interview to explore cuttingedge insights and career advice for early-career researchers in the membrane community!

Amir: Can you tell us about your background, career, and professional journey over the last 10-15 years, starting from your education?

Sebastien: I began with a Bachelor of Chemistry at the University of Nantes in France, completed in 2003, followed by a Master's in Water Chemistry and Microbiology in 2005. From 2005 to 2008, I pursued a PhD at ENSI University of Poitiers, focusing on water chemistry, oxidation processes, and disinfection byproducts, not directly related to membranes.



Sebastien: After a postdoctoral role at CNRS, France's equivalent to CSIRO, I moved to Australia in 2009 to lead a project at Curtin University as a Senior Research Fellow, where I worked for 12 years until 2022. Since 2022, I've been with CSIRO, advancing membranebased solutions for water and resource challenges.

Amir: When and how did you first encounter membrane technology?

Sebastien: My first exposure to membranes was around 2013–2014 at Curtin University. I was working on a project on oxidation processes with ceramic membranes due to their advanced oxidation and catalytic properties. Over time, my work expanded to include nanofiltration and ultrafiltration, and in the last 3–4 years, I've focused on electroseparation technologies, specifically electrodialysis reversal (EDR) and bipolar membrane electrodialysis.

Amir: Can you elaborate on the current state and future potential of bipolar membrane electrodialysis and EDR, especially in the context of their applications?

Sebastien: EDR and bipolar membranes serve distinct purposes. EDR is a mature technology significant potential, especially with in Australia, where climate change drives water scarcity and increasing salinity. It's energyefficient, can be remotely controlled, and integrates well with green energy, making it ideal for remote communities and mining industries aiming for zero liquid discharge. It complements reverse osmosis (RO), which is energy-intensive and less suitable for certain applications. saline water Bipolar membranes, while less commercialised, are transformative for circular economy applications. They enable on-site production of acid and base streams from salt solutions, reducing the need for chemical transport, which is costly in places like Western Australia. They also support resource recovery, such as nutrients from wastewater or metals like lithium in mining, offering additional profit by recovering valuable materials. EDR is more established, but bipolar membranes are gaining traction, particularly for specialised applications.

Amir: What are the main bottlenecks for bipolar membrane technology, and how do they vary by application?

Sebastien: The bottlenecks depend on the application.

Sebastien: For resource recovery, like extracting lithium or ammonia, the challenge is developing selective membranes tailored to specific ions. For example, there's ongoing work on lithium-selective membranes, but ammonia-specific membranes are still lacking, though startups are addressing this. For chemical production, the focus is on stack design to improve energy efficiency. Highsalinity solutions pose issues due to calcium and magnesium precipitation in basic streams, which can be mitigated by pretreatment, such as nanofiltration to remove divalent ions, or by developing monovalent-selective membranes. Research, particularly in Europe, is advancing, with claims of up to 50% energy reduction through innovative stack configurations. The robustness for monovalent technology's membranes isn't fully mature, but future developments will likely address this.

Amir: How do you address concerns about bipolar membranes handling highly saline or high-TDS solutions?

Sebastien: High total dissolved solids (TDS) aren't inherently problematic if the solution is simple, like sodium chloride. The issue arises hardness with ions like calcium and magnesium, which precipitate in the basic stream. This can be tackled by adding a pretreatment step, such as nanofiltration, to selectively remove divalent ions, allowing the to bipolar membrane operate safely. Alternatively, research is exploring monovalent-selective membranes that reject calcium and magnesium, though these are not yet robust or market-ready. I'm optimistic that future membrane designs will resolve these challenges, enabling bipolar membranes to handle high-TDS solutions effectively.

Amir: What advice do you have for earlycareer researchers (ECRs) interested in membrane technology or water/mineral processing, considering paths in academia versus industry? Sebastien: EDR and bipolar membranes are exciting fields, aligning with sustainability goals like zero liquid discharge, circularity, and green energy, particularly in Australia's remote communities and mining sector. These technologies offer modular, lowmaintenance solutions, ideal for large, sparsely populated regions. In academia, you have more freedom to push boundaries and explore novel ideas, though funding often ties you to industry needs. This path suits curious researchers who thrive on experimental uncertainty. Industry, especially in Western Australia, prioritises quick deployment of existing technologies, offering less flexibility but clear targets, which suits those who prefer structured roles.

Amir: If you could go back to your 20-yearold self, just after your bachelor's degree, what advice would you give?

Sebastien: I'd tell myself to better understand the administrative work surrounding research. It's not fun, but it's a reality that takes up a lot of time, especially as you advance to senior roles like tenured positions. Learning to manage admin tasks early—rather than avoiding them, as I did—saves time and lets you focus more on actual research.

Dr. Sebastien Allard's comprehensive insights into EDR and bipolar membrane technologies, coupled with his practical advice for ECRs, inspire the MSA community to advance sustainable solutions for water and resource challenges. Thank you for sharing your expertise and vision!

Smart Synergy: Al and Membranes Transforming Water Infrastructure

BY SHOKAT AKBARNEZHAD, MILTON CHAI



Introduction

As artificial intelligence (AI) continues to transform industrial operations, its integration into water and wastewater treatment is opening new frontiers in process optimisation, energy efficiency, and sustainable resource management. Recent developments highlight how AI technologies are reshaping membrane-based systems at both the system and infrastructure levels. In Singapore, Gradiant is deploying its AIpowered SmartOps platform to enhance energy efficiency in desalination systems system-level through control and prediction. Meanwhile, in the United States, xAI is constructing the world's largest ceramic membrane bioreactor (MBR) to reuse municipal wastewater for cooling a high-performance Al data centre by leveraging advanced ceramic membrane technology delivered by CERAFILTEC. Together, these initiatives signal a shift toward intelligent, scalable, and sustainable membrane operations enabled by AI.

Al-Powered Desalination to Cut System-Wide Energy Use

Gradiant, a global water solutions provider, has secured a €5.4 million grant from Singapore's PUB and the National Research Foundation to develop a low-energy desalination facility at the Desalination Integrated Validation Plant (D-IVP) in Ulu Pandan. The facility will feature SmartOps AI, Gradiant's proprietary machine learning platform, designed to optimise entire water treatment systems rather than isolated components.

The facility will incorporate Gradiant's Smart Operations (SmartOps) Artificial Intelligence (AI) technology-a machine learning-based digital platform designed to optimise overall plant performance rather than focusing only on individual treatment units. While technologies such as ceramic membranes pretreatment and ultra-permeable for membranes for seawater and brackish water reverse osmosis (SWRO and BWRO, respectively) have improved energy efficiency at the component level, SmartOps Al addresses energy optimisation at the fullsystem scale. The AI platform predicts operational needs in real time, including membrane cleaning and replacement, aiming to lower energy consumption to kWh/m³ 2 from the under current benchmark of 3.5 kWh/m³.

The project involves collaboration with the National University of Singapore (NUS), water treatment startup Hydroleap, and the Separation Technologies Applied Research and Translation (START) Centre. The facility is expected to be operational by the end of 2025 and will serve as a model for the future of intelligent, energy-efficient desalination both in Singapore and globally.

Al and Ceramic Membranes Unite for Sustainable Data Center Cooling

In a bold step toward integrating artificial intelligence with sustainable water technology, xAI, an AI company founded by Elon Musk, is constructing what will become the world's largest ceramic membrane bioreactor (MBR) in Memphis, Tennessee, USA.

The facility will treat and recycle 49.2 MLD, equivalent to 13.0 MGD, of municipal wastewater to cool its next-generation supercomputing data centre, scheduled for completion in 2025.

CERAFILTEC, German company a specialising in ceramic membrane technologies, will deliver its most advanced system for this fast-track project. The CERAFILTEC's selection was based on technical capabilities and ability to meet the accelerated timeline.

The project reflects the increasing role of ceramic membrane technology in largescale, critical applications. xAI's wastewater treatment plant will exceed its own cooling needs, supplying additional treated water to local industries, thus reducing pressure on the Memphis Sands Aquifer and supporting sustainable water practices.

xAI aims to ensure a reliable cooling water supply for its AI systems while minimising use of potable water. The project is led by Mark Carroll, xAI's wastewater engineer.

Dr. Torsten Wintergerste, recently appointed CERAFILTEC, CEO emphasised of the alignment between both companies in advancing AI and water treatment. Dr. Juergen Hambrecht, Chairman of CERAFILTEC, stated that this collaboration sets a new industry benchmark in through wastewater reuse ceramic membrane technology.





Figure 1. xAI's Colossus data centre compute hall (top) and CERAFILTEC's ceramic membrane filtration module (bottom). Sources: [1], [2]

About xAI: Headquartered in San Francisco, USA, xAI focuses on advancing scientific discovery through artificial intelligence. Its AI system, Grok, integrates real-time data from the social platform X.

About CERAFILTEC: Based in Germany, CERAFILTEC specialises in ceramic ultrafiltration membrane technology for water and wastewater treatment worldwide.

Sources: [3], [4]



Membrane Society of Australasia



ISSUE NO. 46