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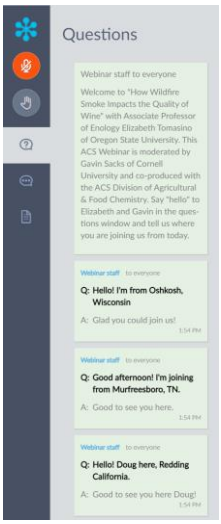

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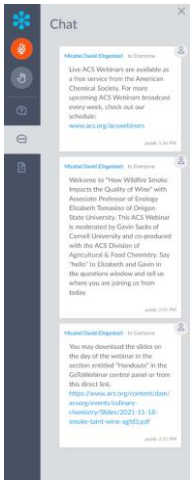
Chat

Announcements and hyperlinks from our team



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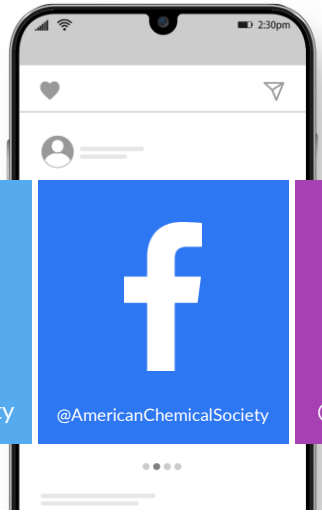

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ChemIDP is an Individual Development Plan designed specifically for graduate students and postdoctoral scholars in the chemical sciences. Through immersive, self-paced activities, users explore potential careers, determine specific skills needed for success, and develop plans to achieve professional goals. **ChemIDP** tracks user progress and input, providing tips and strategies to complete goals and guide career exploration.

https://chemidp.acs.org

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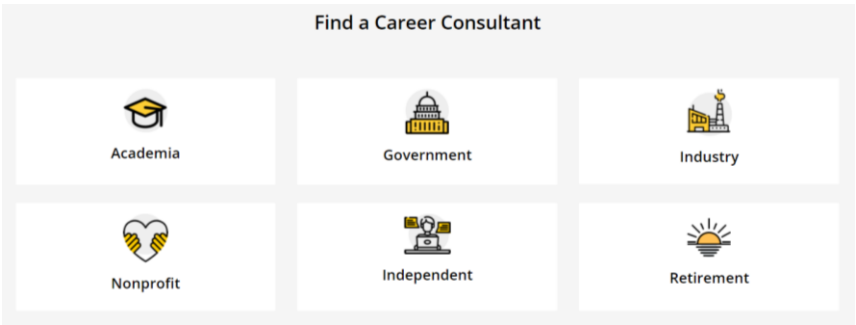
Career Consultant Directory



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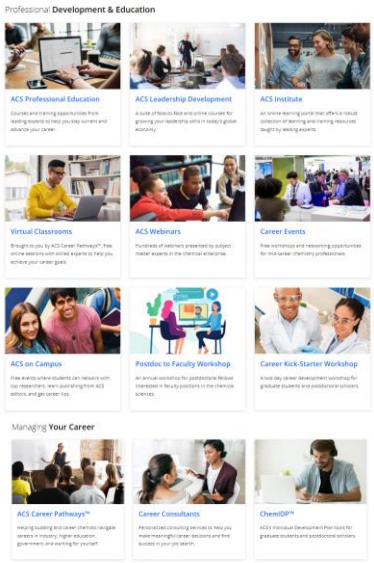
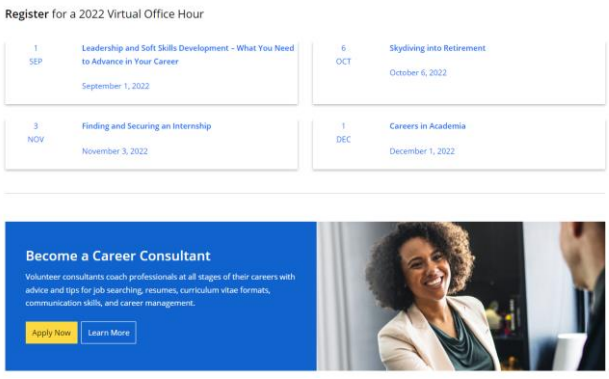
ACS Career Resources





https://www.acs.org/content/acs/en/careers/personal-career-consulting.html

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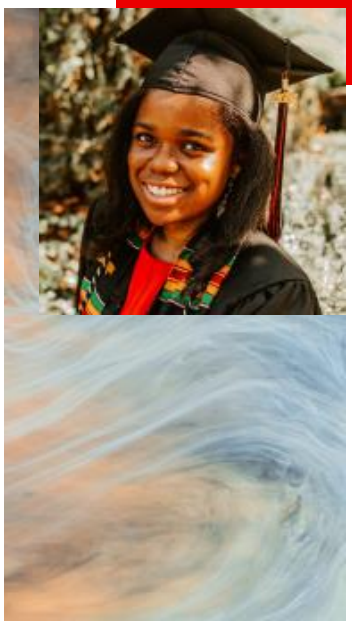

ACS Scholar Adunoluwa Obisesan

BS, Massachusetts Institute of Technology, June 2021
(Chemical-biological Engineering, Computer Science & Molecular Biology)

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Advancing ACS' Core Value of Diversity, Equity, Inclusion and Respect

Resources

Inclusivity Style Guide
Designed to help staff and members use language and images that respect diversity in all its forms.

ACS Webinars on Diversity
Covering diversity and inclusion at the workplace

ACS Publications DEIR Hub
See what ACS Publications is doing for fostering inclusivity in scholarly publishing

ACS Volunteer and ACS Meetings Code of Conduct
Fostering a positive and welcoming environment for attendees, volunteers and staff.

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C&EN highlights scientists from different backgrounds who are making an impact in chemistry.

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Download this educational guide for additional recommendations on videos, articles, books, podcasts, and more on diversity, inclusion, and related topics.

Quick Guide: Inclusion Moments
Learn more about what Inclusion Moments are and see ideas to host them during your meetings.

Quick Guide: How to host inclusive in-person events
Recommendations and best practices to ensure that your events can accommodate everyone.

Diversity, Equity, Inclusion, and Respect
**Adapted from definitions from the Ford Foundation Center for Social Justice:

Equity**
Seeks to ensure fair treatment, equality of opportunity, and fairness in access to information and resources for all. We believe this is only possible in an environment built on respect and dignity. Equity requires the identification and elimination of barriers that have prevented the full participation of some groups.

Diversity**
The representation of varied identities and differences (race, ethnicity, gender, disability, sexual orientation, gender identity, national origin, tribe, caste, socio-economic status, thinking and communication styles, etc.), collectively and as individuals. ACS seeks to proactively engage, understand, and draw on a variety of perspectives.

Inclusion**
Builds a culture of belonging by actively inviting the contribution and participation of all people. Every person's voice adds value, and ACS strives to create balance in the face of power differences. In addition, no one person can or should be called upon to represent an entire community.

Respect
Ensures that each person is treated with professionalism, integrity, and ethics underpinning all interpersonal interactions.

https://www.acs.org/content/acs/en/about/diversity.html

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ACS Green Chemistry Institute
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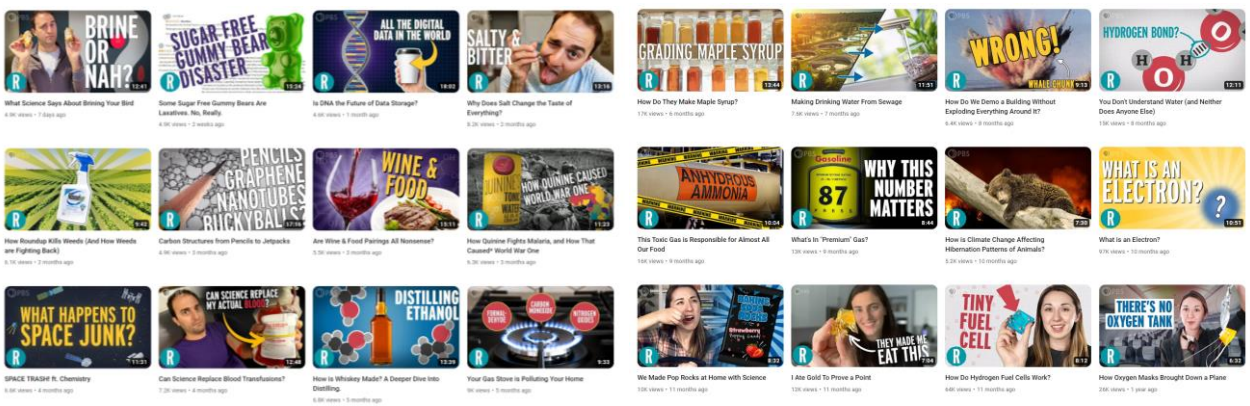

https://www.youtube.com/c/ACSReactions/videos

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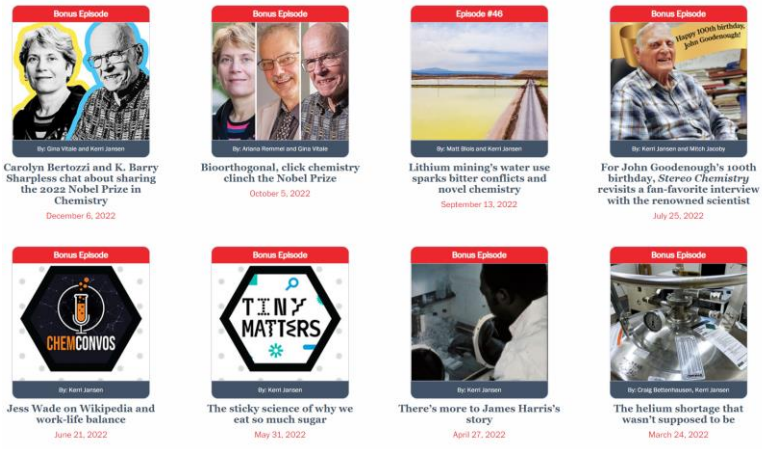
c&en's STEREO CHEMISTRY



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Electrochemical Wastewater Refining: Converting Pollutants into Products

WILLIAM TARPEH, PhD

Assistant Professor of Chemical Engineering, Stanford University

MARK JONES, PhD

Creative Director, MJPhD, LLC

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Electrochemical Wastewater Refining: Converting Pollutants into Products

William Tarpeh
January 19, 2023
ACS Webinar

Stanford | ENGINEERING
Chemical Engineering

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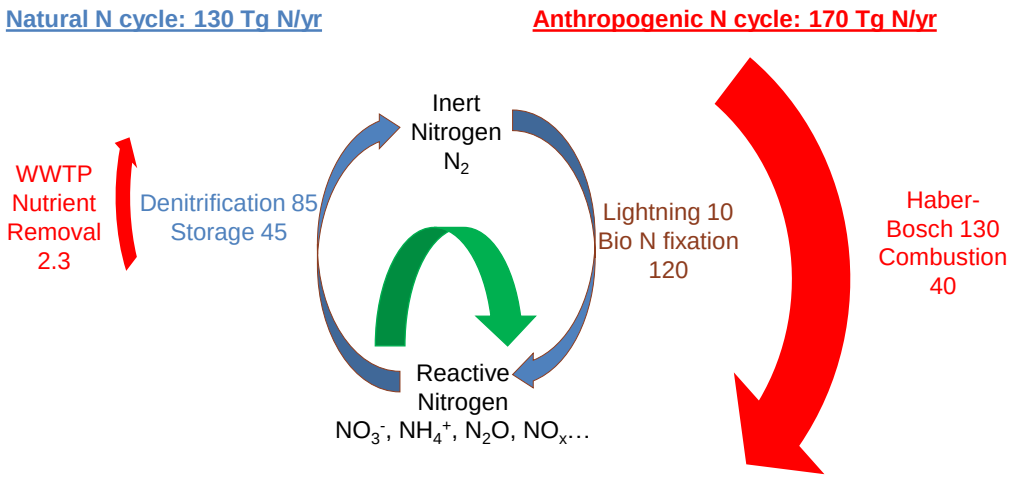
Conventional chemical extraction, manufacturing, and disposal have exceeded planetary boundaries.

> Pollution is nothing but the resources we are not harvesting. We allow them to disperse because we've been ignorant of their value.
> *-R. Buckminster Fuller*

J. Lokrantz/Azote based on Steffen et al. 2015.

The nitrogen cycle is overdue for a 21st century redesign.



$$NO_3^- + 10H^+ + 8e^- \rightarrow NH_4^+ + 3H_2O$$

Data from Fields 2004. Env Health Perspectives

Current nitrogen management poses environmental and equity challenges

Environmental

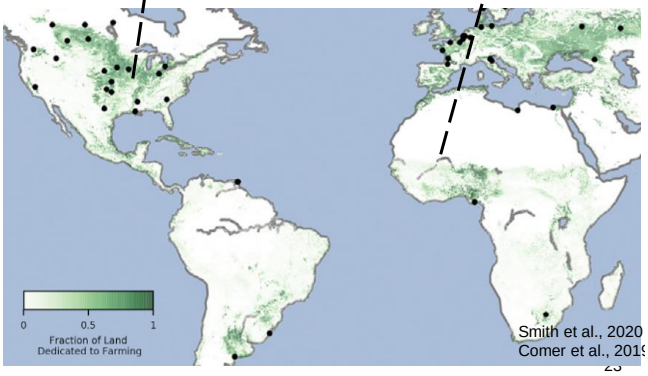
119 Mt aqueous N pollution

320 Mt CO_2 emitted

Equity

US
$550/tonne N
$66k GDP/capita

Mali
$1106/tonne N
$2.4k GDP/capita



Smith et al., 2020
Comer et al., 2019

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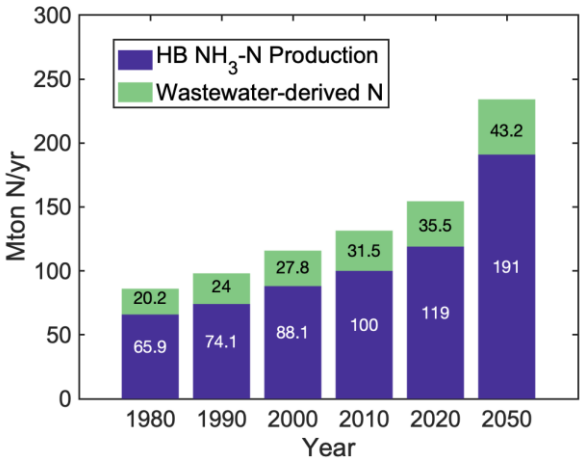
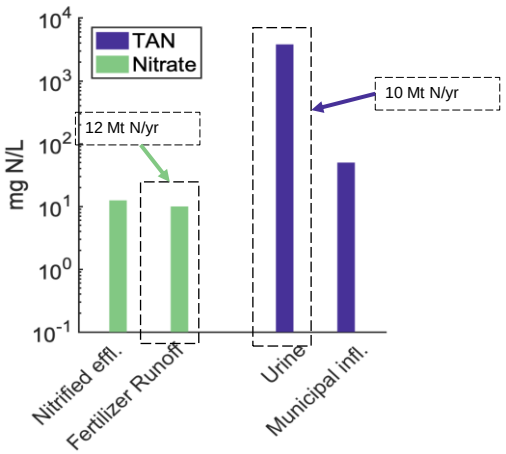
Wastewater nitrogen can substantially offset Haber-Bosch



30% of total Haber-Bosch N can be recovered from fertilizer runoff and municipal wastewater



Both ammonia and nitrate-polluted wastewaters present opportunities

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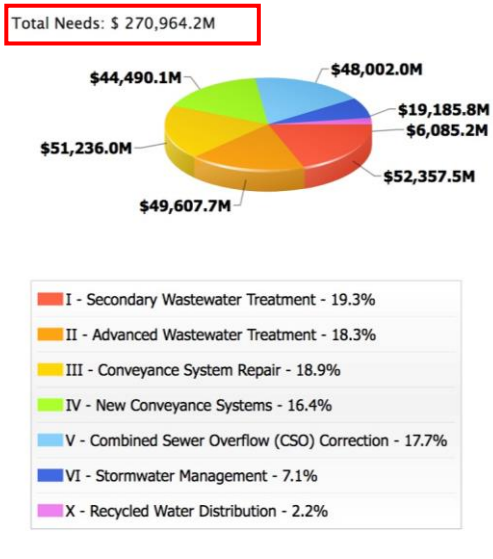
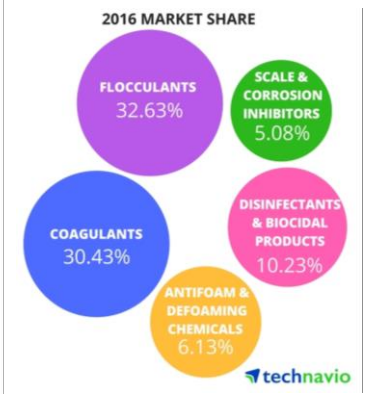
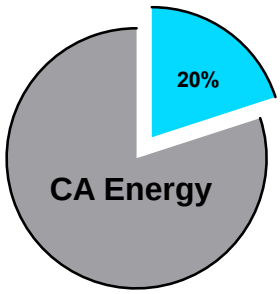
Treating wastewaters requires money, energy, and chemical inputs.







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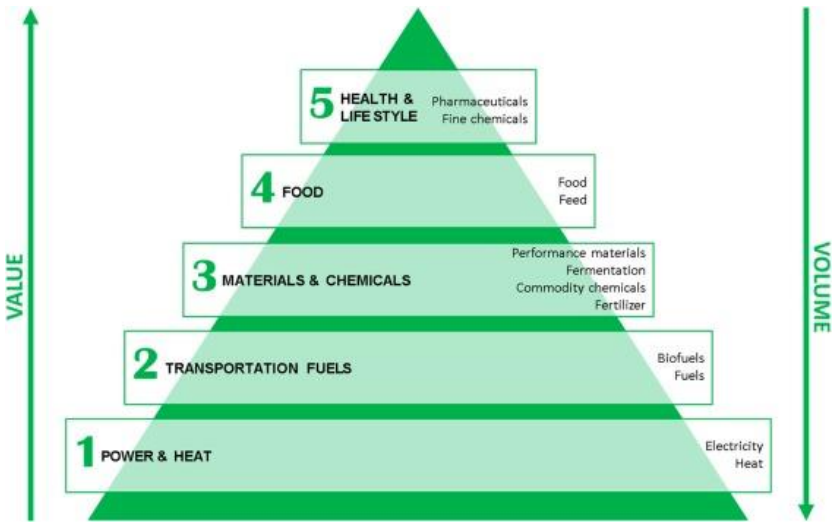
Wastewaters contain valuable chemical resources.



van der Hoek et al., Resources, Conservation and Recycling (2016)

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Audience Survey Question

ANSWER THE QUESTION ON THE INTERACTIVE SCREEN IN ONE MOMENT

What is the most valuable type of wastewater?

- **Reverse osmosis concentrate**
- **Municipal wastewater**
- **Fertilizer runoff**
- **Lithium-ion battery leachate**
- **Geothermal brine**

* If your answer differs greatly from the choices above **tell us in the questions window!**

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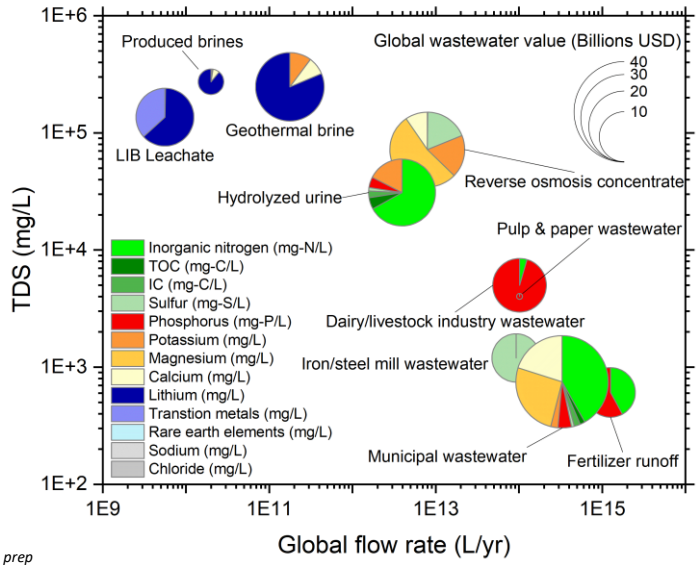
Wastewater refining is the next frontier of pollution mitigation.



Miller, Abels, Guo, Williams, Liu, Tarpeh, in prep

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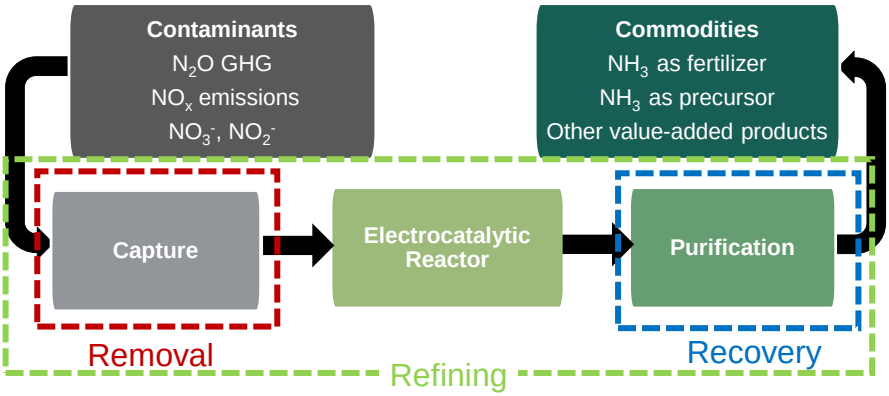
Co-designing catalysis and separations as **reactive separations** can achieve wastewater refining using minimal inputs.



Use separations to control catalytic microenvironments
Valorize feedstocks that degrade in quality
Design multifunctional or cascading reactors

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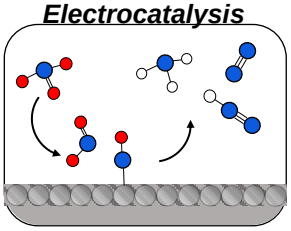
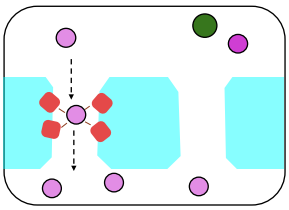
Electrochemical Wastewater Refining Tools

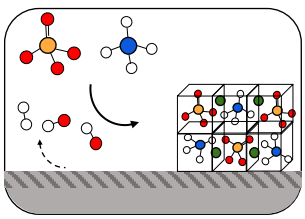
Electrocatalysis



Electrochemical separations



Stoichiometric electrochemical conversions



Modular (flexible-scale)
Integration with renewable energy
Facile process control
Replacing chemical inputs with electricity

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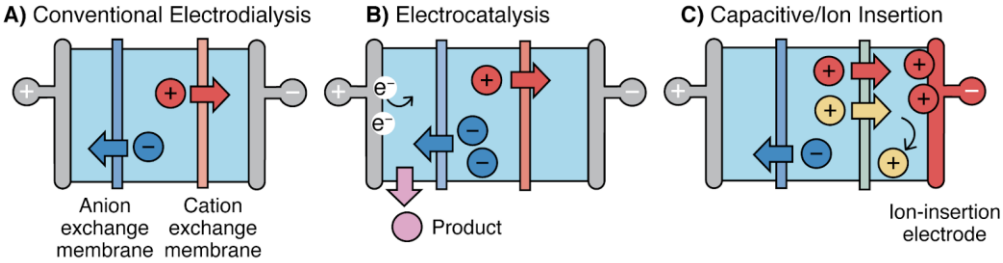
Envisioning Electrochemical Wastewater Nitrogen Refineries



Nitrogen Oxidation State

$NO_3^- + 10H^+ + 8e^- \rightarrow NH_4^+ + 3H_2O$ Reduction

–3	–2	–1	0	+1	+2	+3	+5
Ammonia NH_3	Hydrazine N_2H_4	Hydroxylamine NH_2OH	Nitrogen N_2	Nitroxyl HNO	Nitric oxide NO	Nitrite NO_2^-	Nitrate NO_3^-

Oxidation $NH_3 + 9OH^- \rightarrow NO_3^- + 6H_2O + 8e^-$

Tarpeh and Chen. *Environmental Science & Ecotechnology (2021).*

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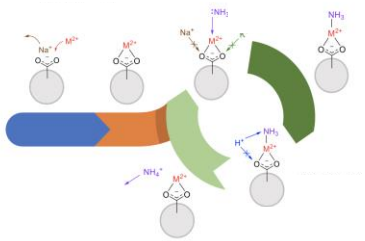
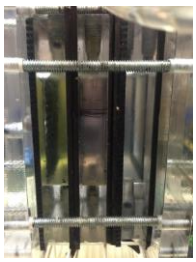
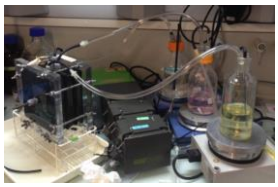
Tarpeh Lab: Designing Reactive Separations + Wastewater Refining

Selective Materials

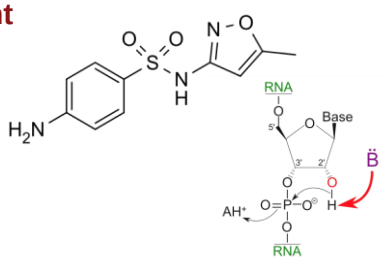




Electrochemical processes



Contaminant fate



Resource-constrained communities

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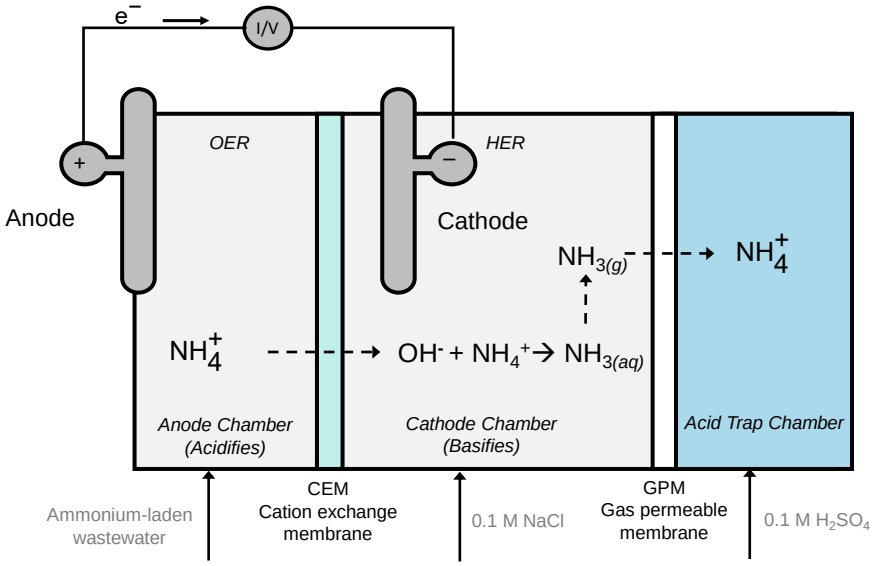
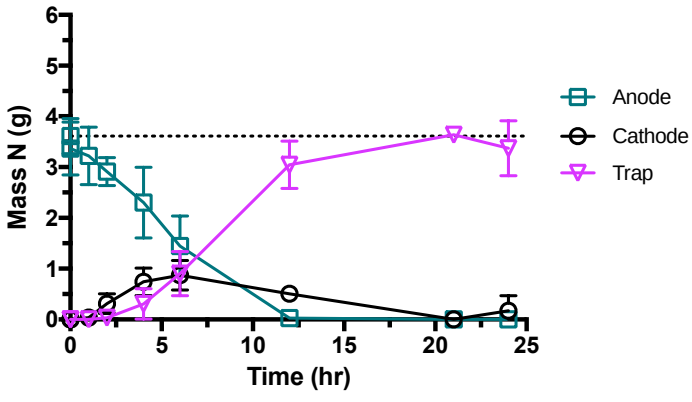
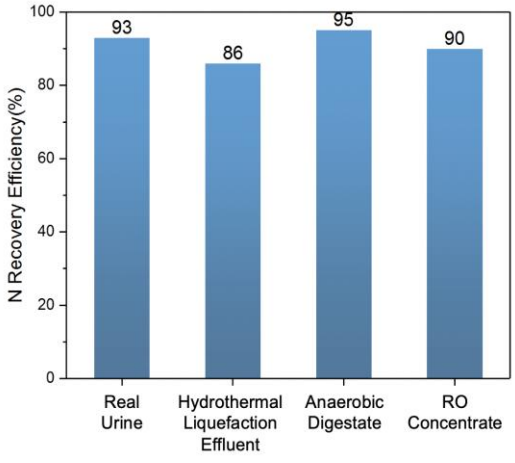
Electrochemical stripping selectively recovers nitrogen from wastewaters based on charge and volatility.



Proof-of-concept: Nitrogen is recovered to the trap chamber





Tarpeh, Barazesh, Cath, Nelson (2018), Environmental Science & Technology.
Li, Tarpeh, Nelson, Strathmann. (2018). Environmental Science & Technology.
Liu, Neo, Tarpeh (2020). Water Research.

Electrodialysis and Nitrate Reduction (EDNR) uses dynamic bias to mitigate ammonia and nitrate pollution by recovering both as ammonia.

NH_3 Recovery

$$NH_4^+ + HO^- \rightleftharpoons NH_3 + H_2O$$

NH_3 Synthesis

$$NO_3^- + 9H^+ + 8e^- \rightarrow NH_3 + 3H_2O$$

Switch E_1 to E_2

Dynamic Bias

Switch E_2 to E_1

Matthew Liu,
PhD student

Jinyu Guo,
PhD student

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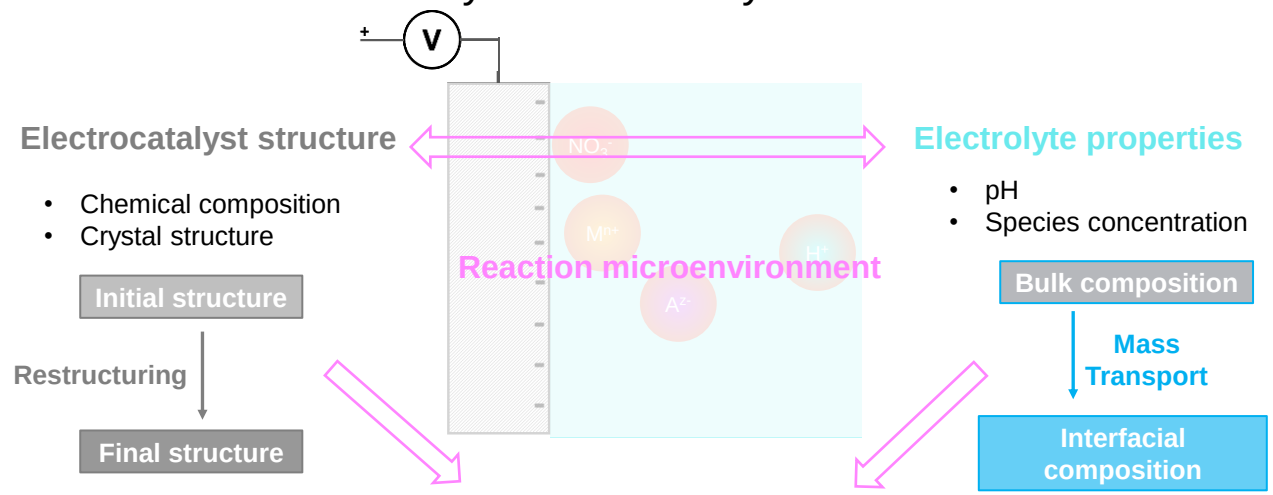
Both sides of the electrocatalyst-electrolyte interface influence electrochemical activity and selectivity.



NO_3RR activity and selectivity

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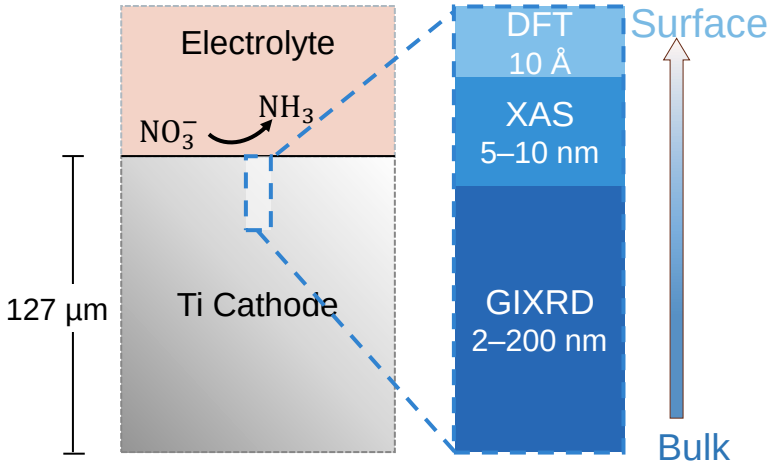
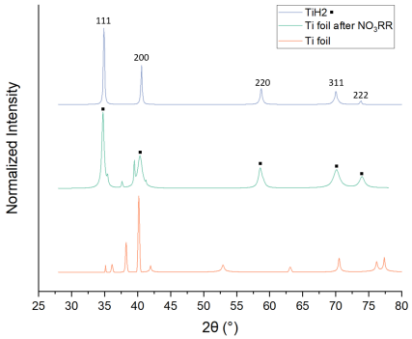
Characterizing an optimal nitrate reduction **electrode**

- Investigate **post NR surface structure** with combined spectroscopy and computation
- **Control in-situ electrochemical TiH_2 formation** via NR applied potential and duration
- Identify **TiH_2 as predominant species**



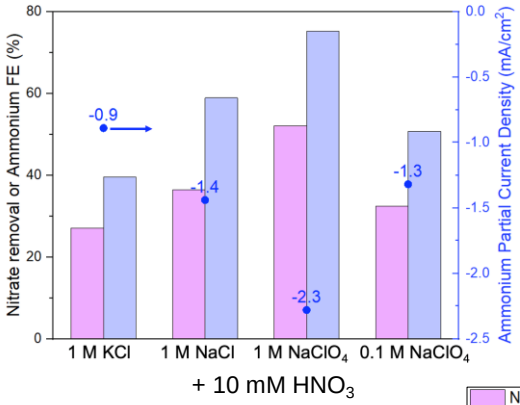
	2 hr	4 hr	6 hr	8 hr
-0.6 V_{RHE}				
-0.8 V_{RHE}				
-1.0 V_{RHE}				



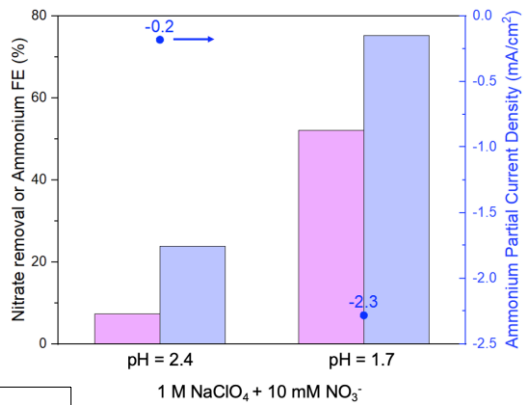
M. J. Liu, J. Guo, A. S. Hoffman, J. H. Stenlid, M. Tang, E. Corson, K. H. Stone, F. Abild-Perdersen, S. R. Bare and W. A. Tarpeh, *JACS* (2022).

Characterizing an optimal nitrate reduction **electrolyte**

- Cation: $Na^+ > K^+$
- Anion: $ClO_4^- > Cl^-$
- Concentration: 1 M > 0.1 M



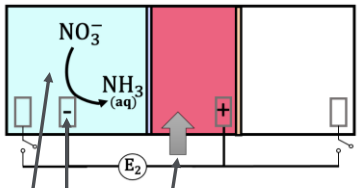
- pH < 2 is crucial for NR activity and ammonia selectivity



Ti foil, -1 V vs. RHE

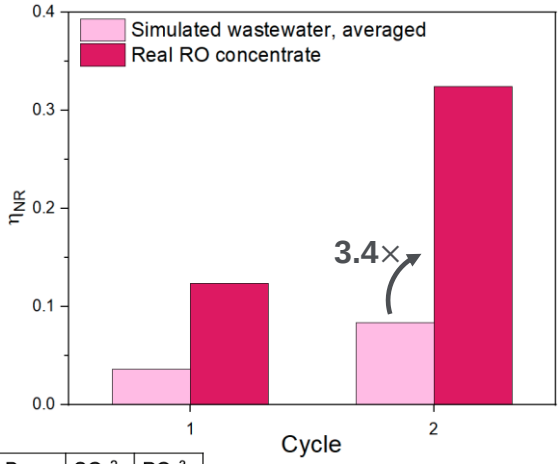
Applying EDNR to real wastewater treatment

Engineered NR microenvironment



- NR electrolyte: 0.1 M $KClO_4$ → 1 M $NaClO_4$, Left chamber pH = 1.8 before starting NR
- NR electrode: Ti → TiH_2/Ti
- Influent: real RO concentrate (50 ppm NH_4^+ + 85 ppm NO_3^-)

Validation with real wastewater



Ion identity	NH_4^+	K^+	Na^+	Ca^{2+}	Mg^{2+}	NO_3^-	Cl^-	Br^-	SO_4^{2-}	PO_4^{3-}
Concentration (ppm)	49	110	784	366	123	85	1396	10	1898	46

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1 Intro | 2 Electrocatalysis | 3 Electrochemical separations | 4 Closing | 5 Closing

Opportunities and Barriers for Homogeneous Catalysis for Wastewater Treatment

Barriers

1. Requires separation
2. Mass transport limitations
3. Scaling up challenges

Opportunities

1. High product selectivity
2. Well-defined active site
3. Integration with separations

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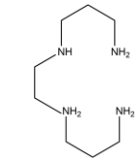
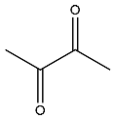
Co-DIM is an ammonia-selective NO_3RR molecular catalyst



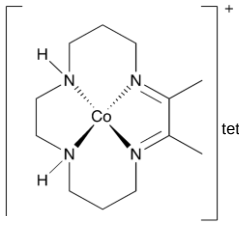
1,2-Bis(3-aminopropylamino)ethane



butanedione

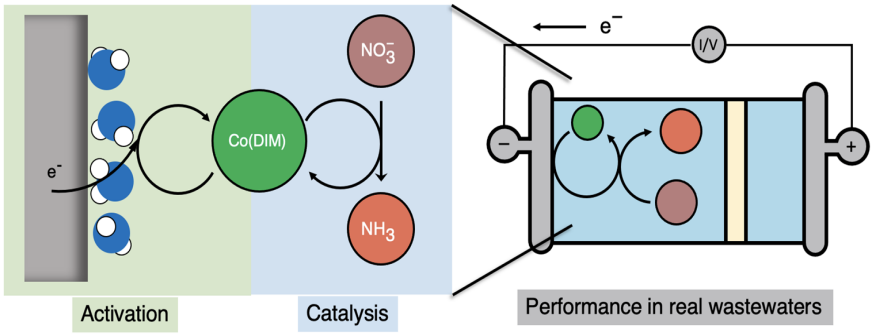
1. 2 eq. HBr, 1 eq. $Co(OAc)_2$, stir under N_2
2. Excess HBr, bubble air
3. Excess $HClO_4$

Methanol



Co-DIM

Co center at 2,3-dimethyl-1,4,8,11-tetraazacyclotetradeca-1,3-diene (DIM) ligand



Matthew Liu, PhD student

Dean Miller, PhD student

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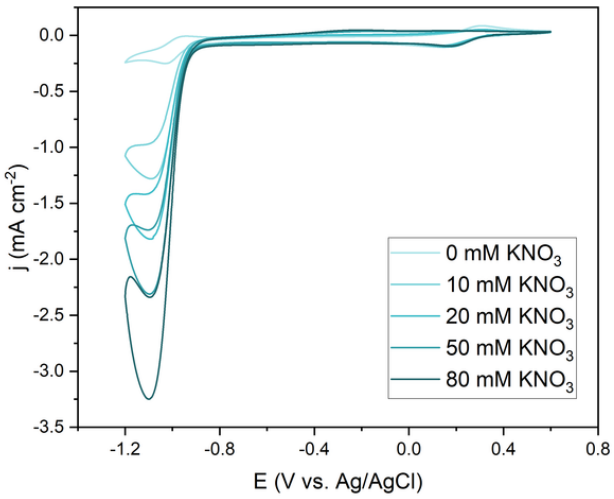
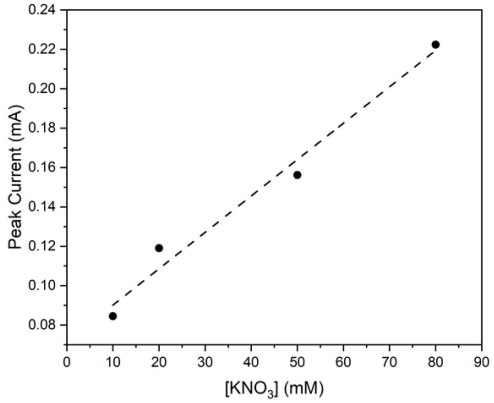
Substrate titration demonstrates the first-order nature of NO_3RR on Co-DIM.



Liu, Miller, Tarpeh, in prep



0.1 M KClO4
2 mM CoDIM
pH 3.7
Ar-purged and blanketed
Polished glassy carbon (3 mm disk)
Graphite rod counter in glass chamber with porous frit
Calibrated 3 M KCl Ag/AgCl reference electrode

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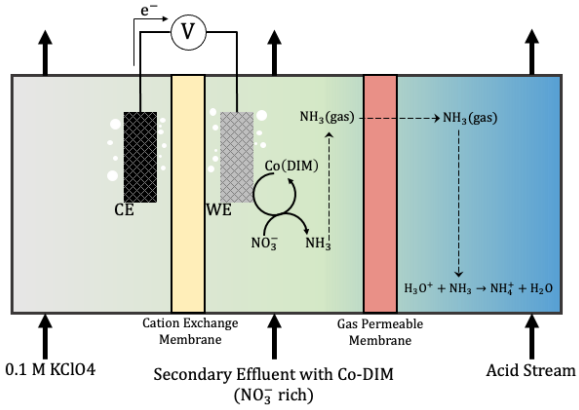
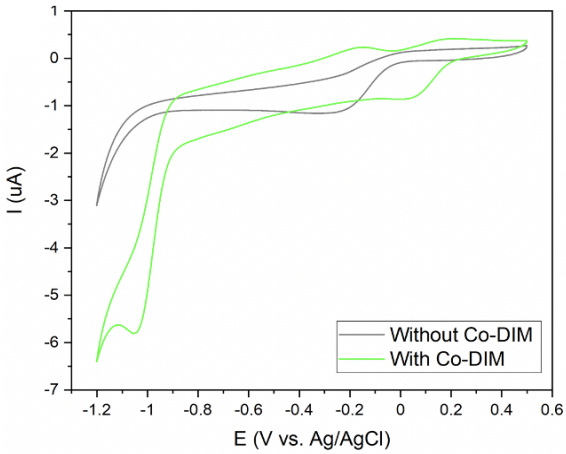
Reactive separations highlight benchmarks for wastewater refining

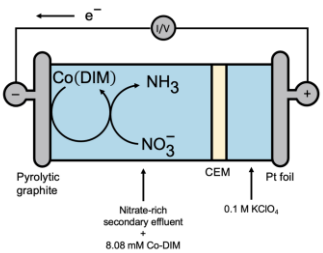


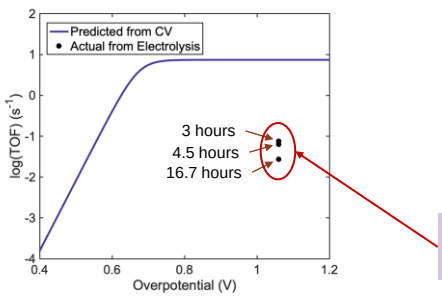
Electrochemical Stripping (ECS)

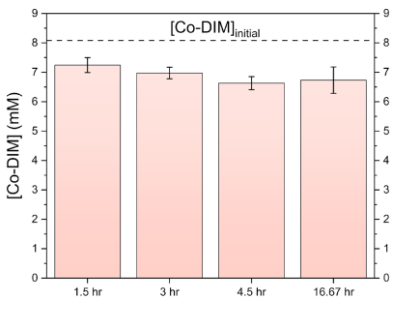


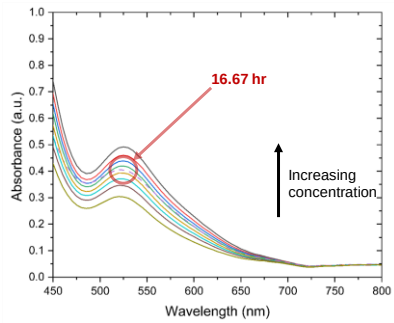
Co-DIM mediated NO_3RR in ECS: 0.344 kWh/g-N
Conventional NDN + HB: 0.025 kWh/g-N

Foot-of-the-wave analysis can also be used as an *in situ* catalyst monitoring tool









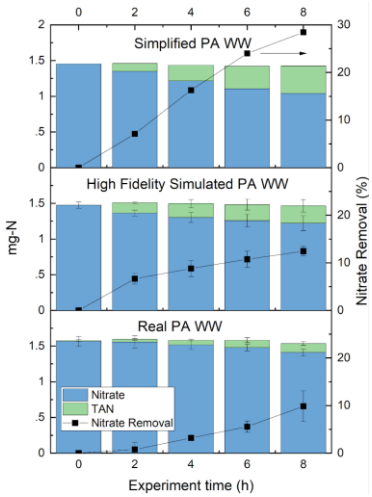
16.67 hr [Co-DIM] from FOWA
6.73 ± 0.45 mM

8.2% error

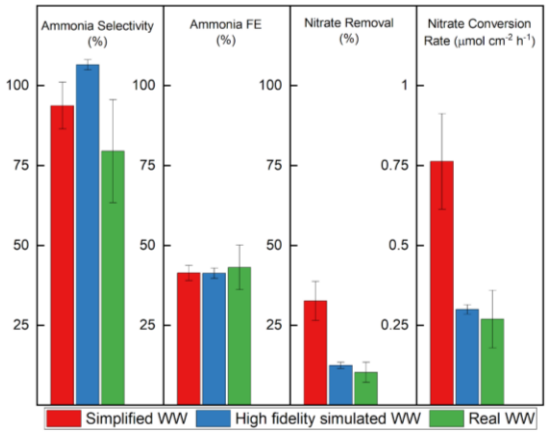
16.67 hr [Co-DIM] from UV-Vis
6.22 mM

Catalyst deactivation is one contributing factor to performance losses in real wastewaters

Wastewater composition influences NO_3RR activity more than selectivity.



	Simplified WW	Simulated WW	Real WW
Nitrate (mg N/L)	28	28	28
Chloride (mg/L)	217	242	228
Bicarbonate (mg/L)	-	84	79
Sulfate (mg/L)	-	106	102
Sodium (mg/L)	-	120	120
Potassium (mg/L)	-	20	20
Magnesium (mg/L)	-	36	36
Calcium (mg/L)	-	76	77
pH	6.50	8.55	8.30
pH (with 8 mM Co-DIM)	3.06	3.42	3.58



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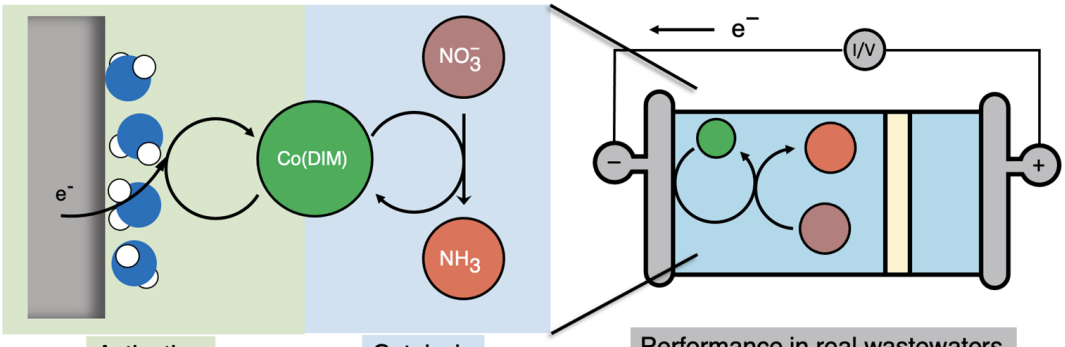
Takeaway: Molecular catalysts can be characterized and integrated in reactive separations that treat real wastewater.



Activation

Co-DIM activates by outer sphere electron transfer

Catalysis

NO_3RR catalysts can be benchmarked and characterized in ECS

Performance in real wastewaters

Quantifiable catalyst degradation contributes to transient activity loss in electrolysis

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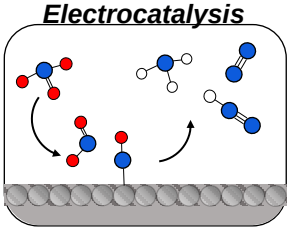
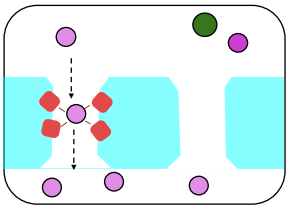
Electrochemical Wastewater Refining Tools

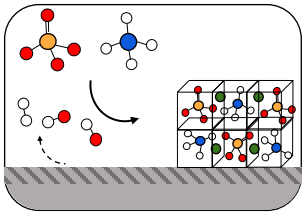
Electrocatalysis



Electrochemical separations



Stoichiometric electrochemical conversions



Modular (flexible-scale)
Integration with renewable energy
Facile process control
Replacing chemical inputs with electricity

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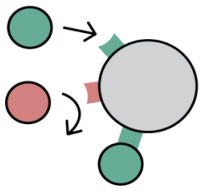
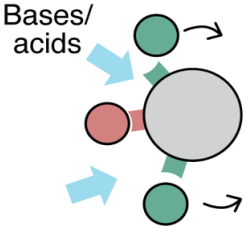
Separations play critical roles in electrochemical wastewater refining

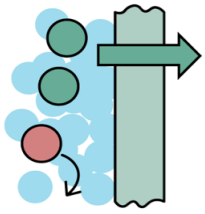
Adsorbent

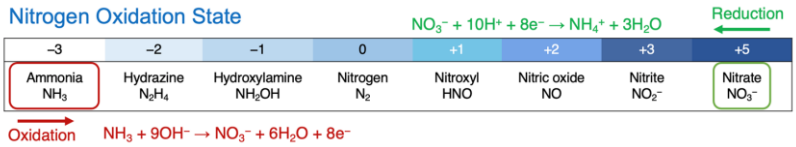


Regenerative Adsorbent



Membrane





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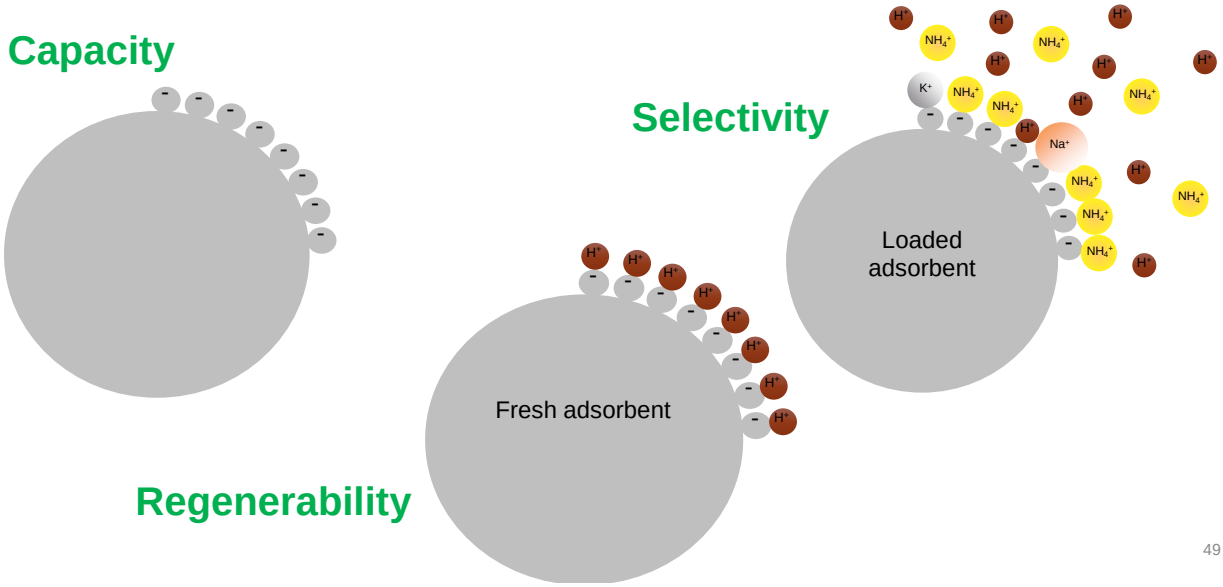
Criteria of an ideal resin for selective aqueous separations



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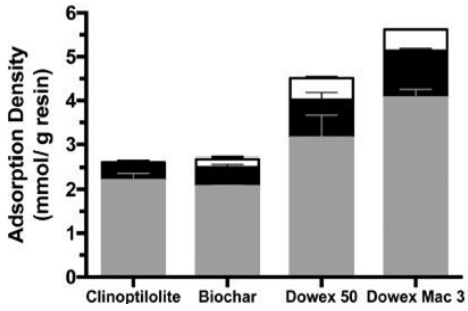
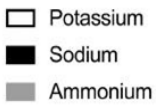
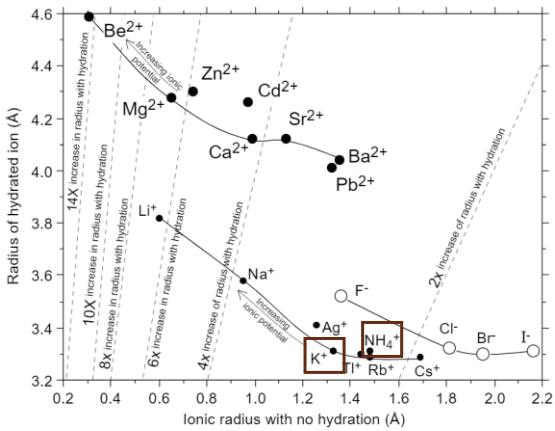
Selectivity depends on the material and solution.





Observed selectivity: majority of sites occupied by N due to urine composition



Intrinsic selectivity: equimolar solutions

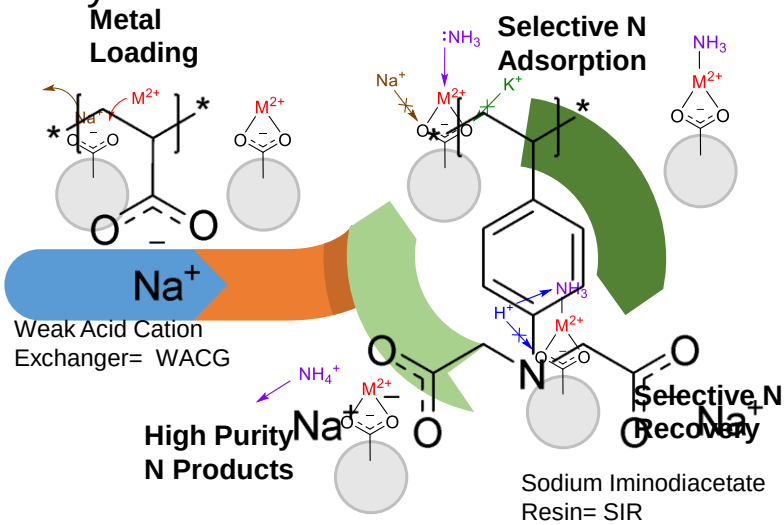
$$\frac{[NH_4^+]_{resin}[K^+]_{aq}}{[NH_4^+]_{aq}[K^+]_{resin}}$$

Tarpeh et al. 2017, Environmental Science & Technology

50

Transition metal-loaded resins can achieve selective nitrogen recovery.

Brandon Clark, PhD student



Clark and Tarpeh (2020), Chemistry: A European Journal

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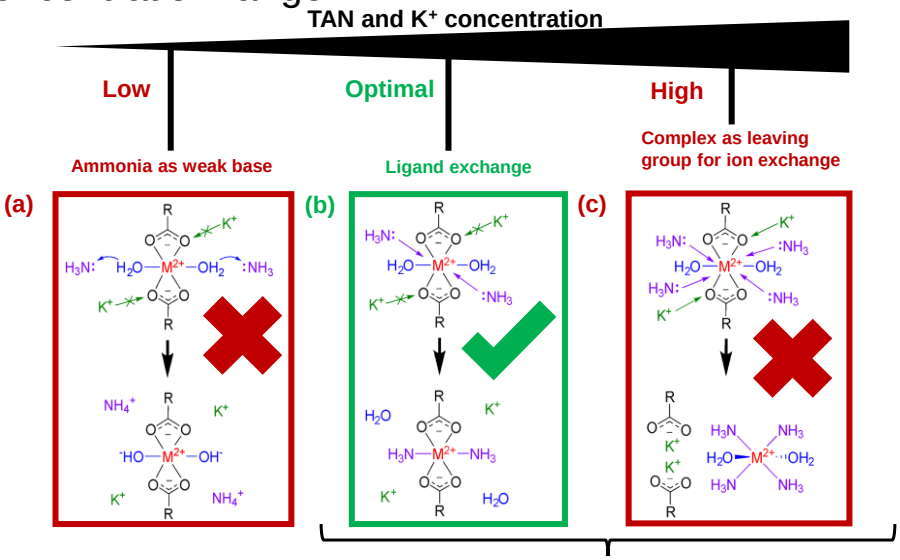
Achieving selectivity with ligand vs. ion exchange introduces an optimal concentration range.



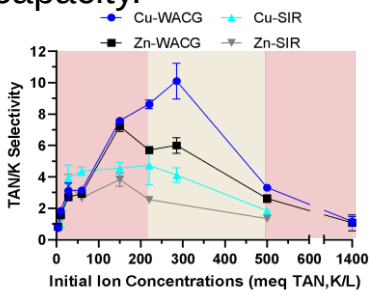
Shifts depending on resin mass per solution volume

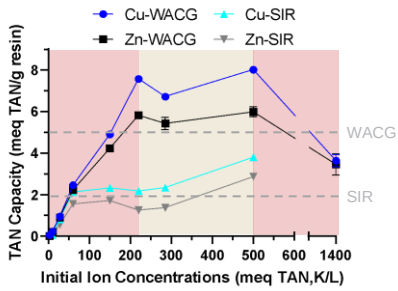
52

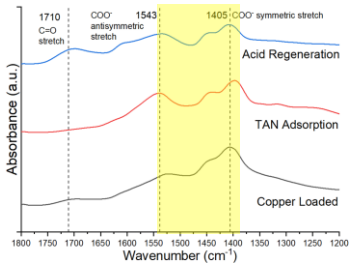
Clark and Tarpeh (2020), Chemistry: A European Journal

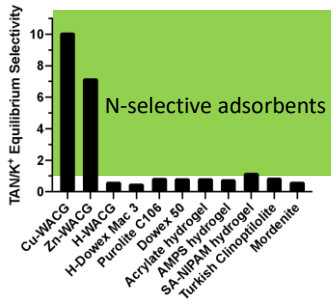
52

Metal-loaded resins achieve unprecedented nitrogen selectivity without sacrificing capacity.









Clark and Tarpeh (2020), Chemistry: A European Journal

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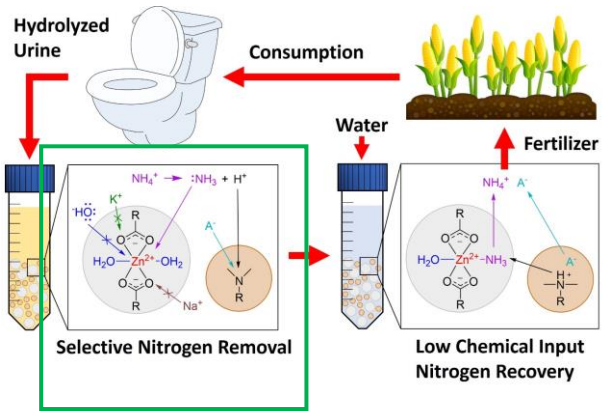
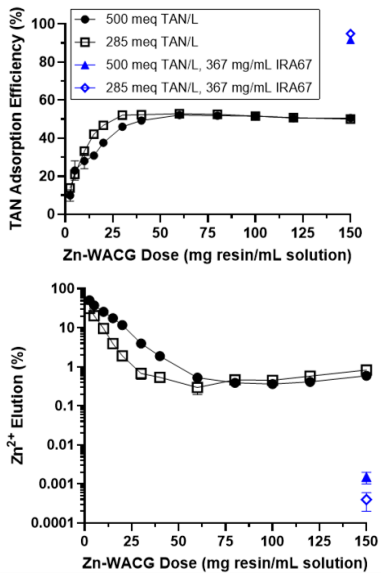
Resin-mediated pH control enhances adsorption efficiency and minimizes zinc elution.





Clark, Gilles, Tarpeh (2022), ACS Applied Materials & Interfaces

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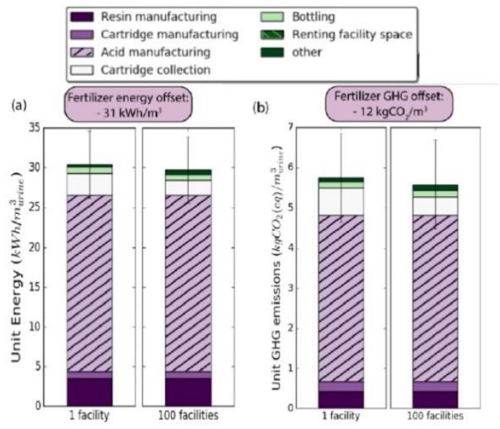
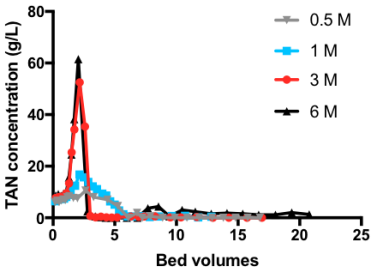
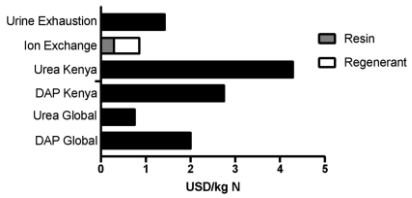
Adsorbent regeneration is a critical part of material and process design.



Sulfuric acid dominates energy and greenhouse gas emissions.[1]



Regenerant concentration influences product concentration and volume.[2]



Regenerant dominates cost in decentralized installations.[3]

1. *Kavvada, Tarpeh, Nelson, Horvath (2017), Environmental Science & Technology*
2. *Tarpeh et al. (2018), Environmental Science: Water Research & Technology*
3. *Tarpeh et al. (2018), Development Engineering*

55

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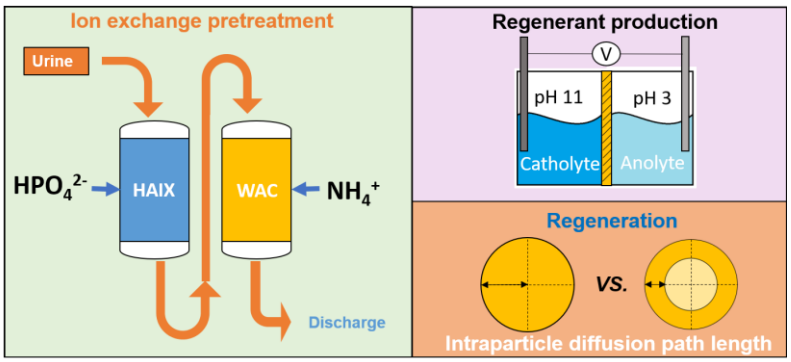
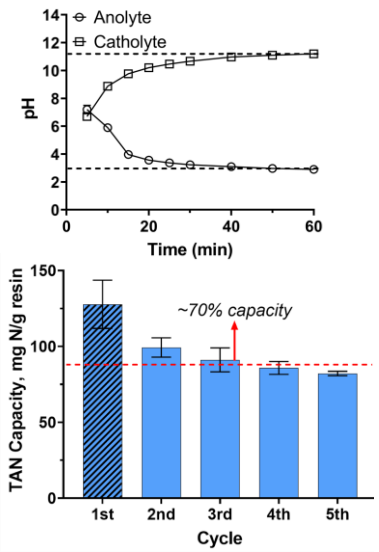
Hang (Lucas) Dong, Postdoc

Electrochemical regeneration can reduce energy and chemical inputs for adsorption.





Dong, Wei, Tarpeh (2020), Water Research.
Dong, Wu, Liu, Tarpeh (2021), Chemical Engineering Journal

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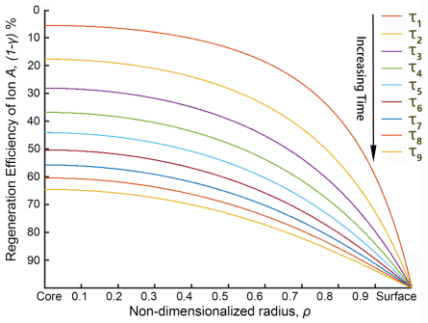
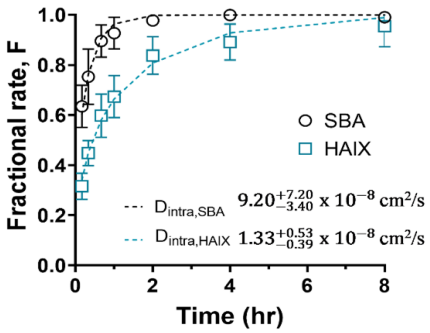
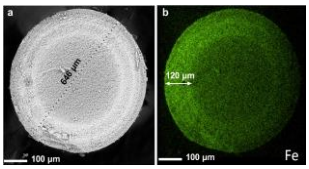
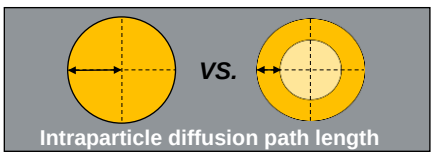
Intraparticle diffusion path length and diffusivity dictate regeneration kinetics.









Dong, Wu, Liu, Tarpeh (2020), Chemical Engineering Journal.

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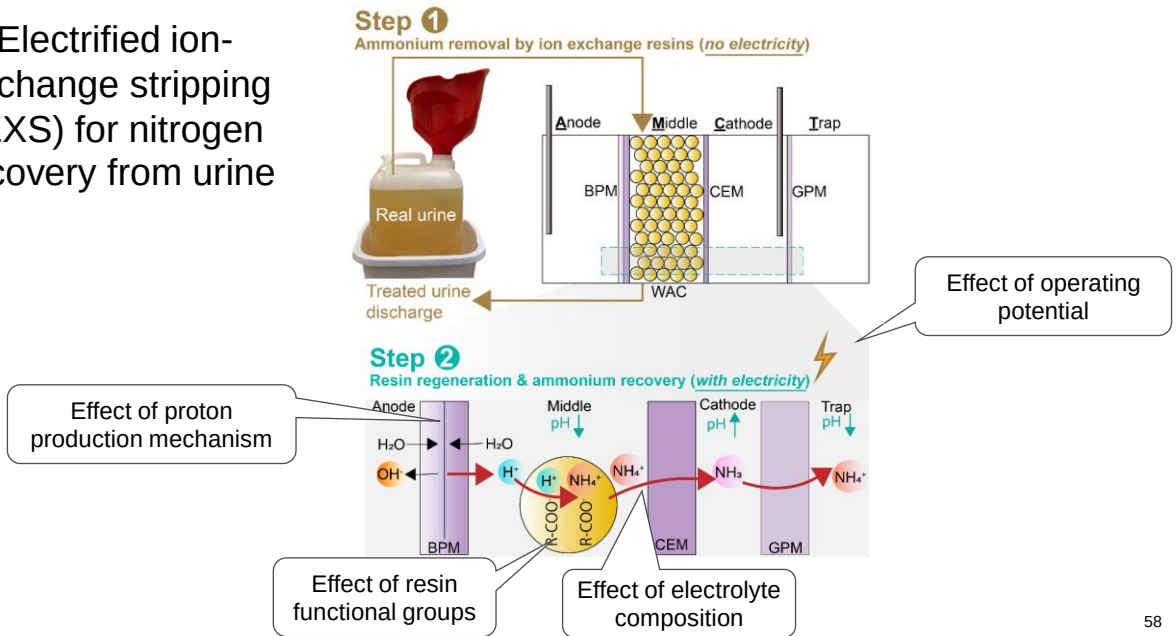
Electrified ion-exchange stripping (EXS) for nitrogen recovery from urine



Dong, Laguna, Liu, Guo, Tarpeh (2022). Environmental Science & Technology.

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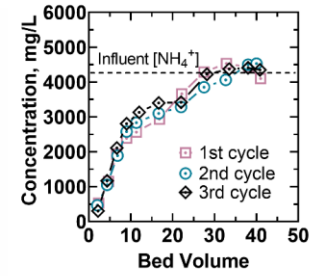
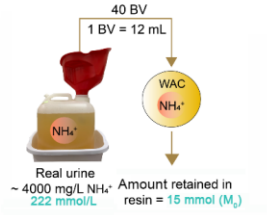
EXS exhibits selective, tunable separation of ammonia from real urine.





- Ongoing: regeneration of ammonium-loaded metal-ligand exchangers
- Future: applications to phosphate for combined N and P recovery

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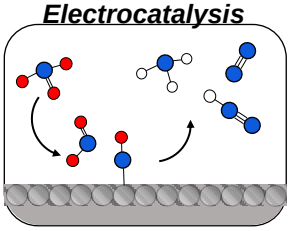
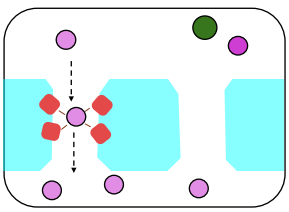
Electrochemical Wastewater Refining Tools

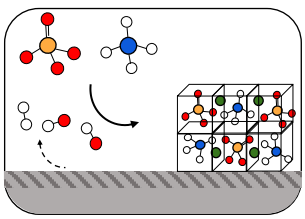
Electrocatalysis



Electrochemical separations



Stoichiometric electrochemical conversions



Modular (flexible-scale)
Integration with renewable energy
Facile process control
Replacing chemical inputs with electricity

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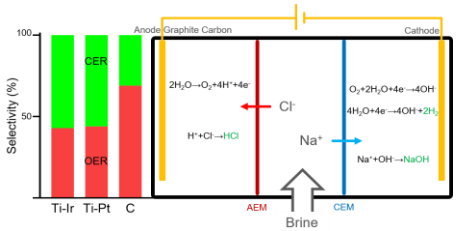
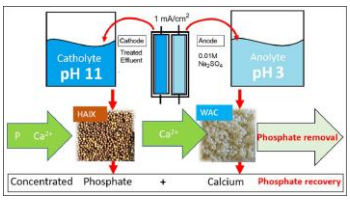
Wastewater refining can achieve element-specific circular economies.

Chemical Production from Desalination Brine



Mu, Wang, Tarpeh (2020), ACS Sus. Chem.

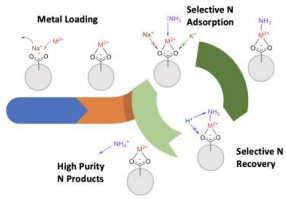
Electrochemical-Adsorption Phosphorus Recovery



Dong, Wei, Tarpeh (2020), Water Research
Dong, Wu, Liu, Tarpeh (2021) Chem Eng. J.

Nitrogen-Selective Adsorbents

Clark and Tarpeh (2020), Chem. Eur J.
Clark, Gilles, Tarpeh (2022), ACS App. Mat.

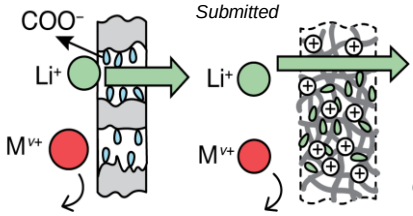


Electrochemical Ammonia Sensors

Lalwani et al., (2021) AIChE Journal

Lithium Recovery from Spent Batteries

Machala, Chen*, Bunke* et al. Submitted*



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1 Intro | 2 Electrocatalysis | 3 Electrochemical separations | 4 Closing | 5 Closing

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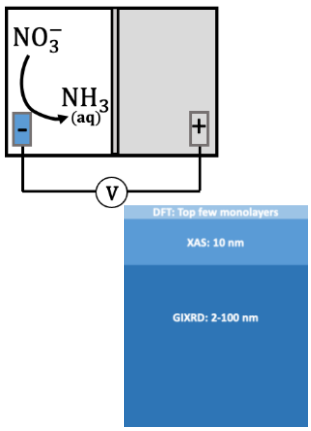
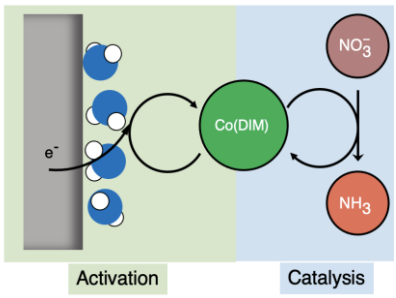
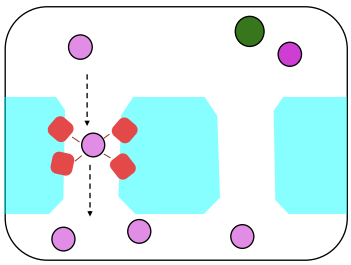
Questions?



Any useful statement about the future should at first seem ridiculous. *-Jim Dator*





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