16th STS-AIChE Southwest Process Technology Conference

- Electrocatalysis with MNenes
- Abdoulaye Djire
- Texas A&M University

Sept 22-23, 2025, University of Houston

16th STS-AIChE Southwest Process Technology Conference

Speaker Bio

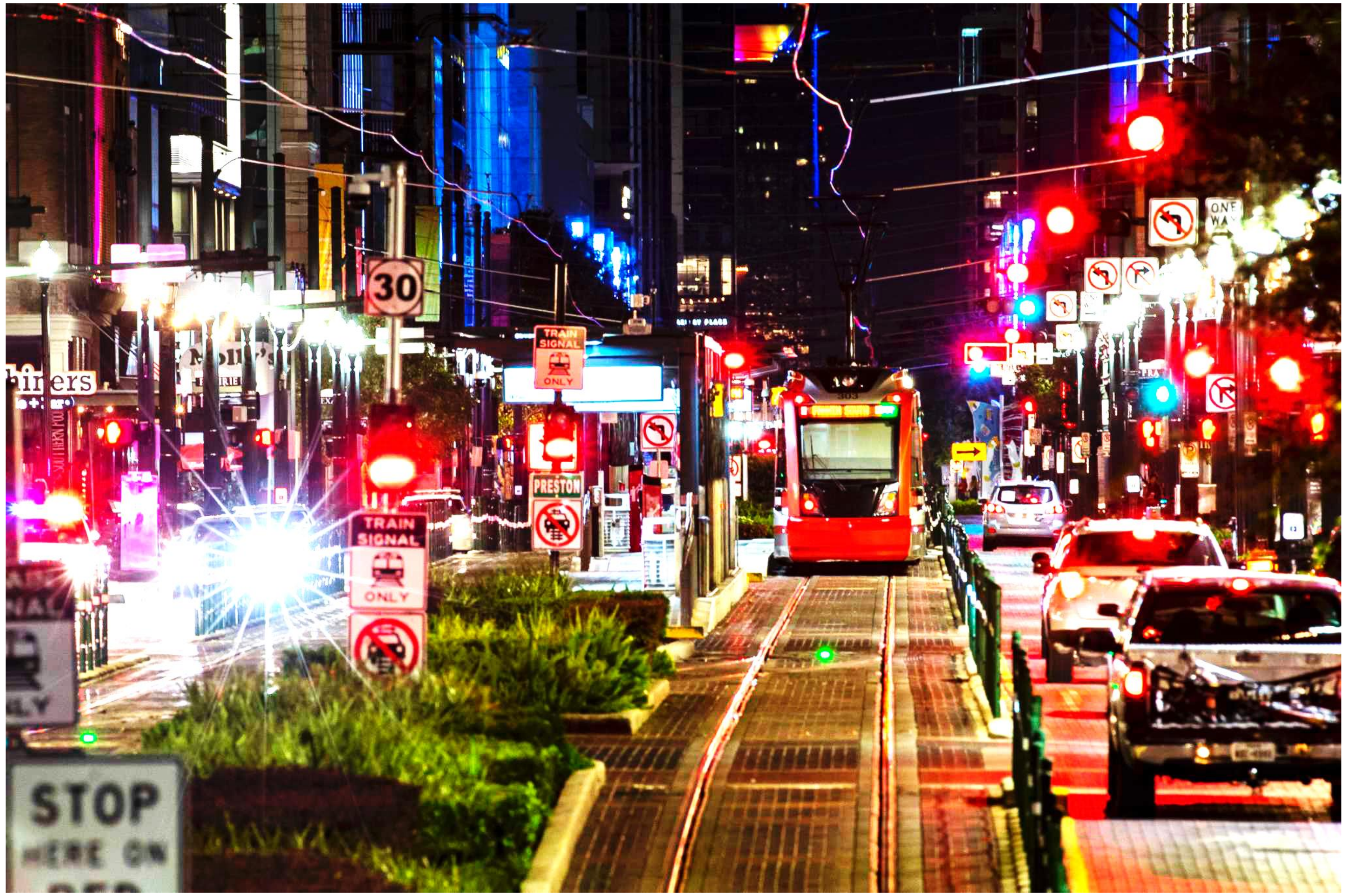
Dr. Djire is an expert in the synthesis and characterization of 2D materials and is considered as one of the pioneers of 2D nitride MXenes. Dr. Djire has published over 40 research articles since joining the Texas A&M faculty and has delivered numerous invited talks at prestigious institutions and international conferences. Dr. Djire has received numerous awards and recognitions including the DOD ARO Early Career Award, the DOE ARPA-E SPARKS Award, the DuPont GOLD Award, and the U.S.-Africa Frontiers Fellowship. Internally, he has received the College of Engineering Dean's Excellence Award and his department's Outstanding Junior Faculty Award, both of which recognize his teaching as well as research excellence.

Sept 22-23, 2025, University of Houston

Houston

1960

2024

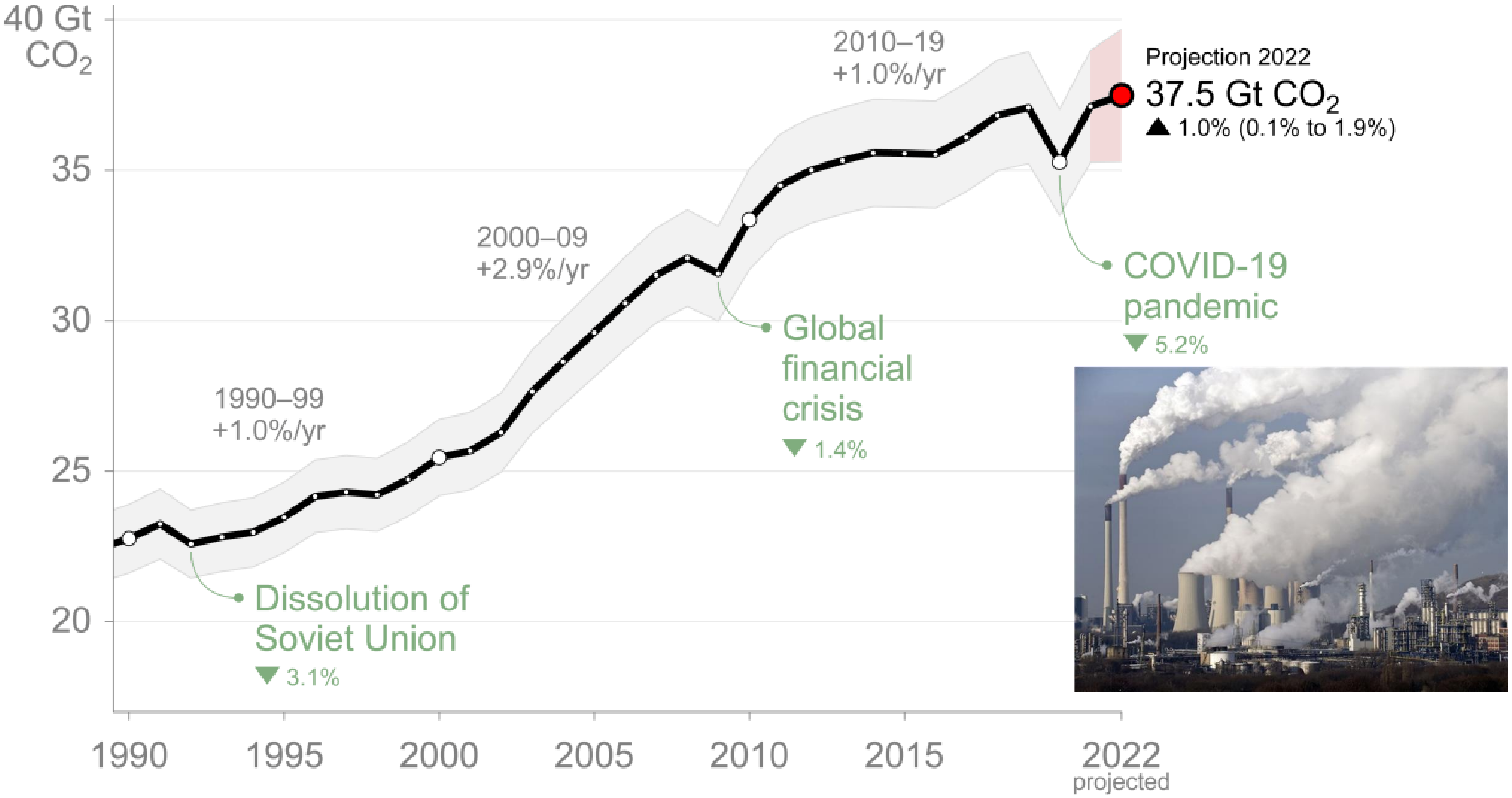


A Global Problem

Bamako

Dakar

Global Fossil CO_2 Emissions Trend



Green Car Congress—The Global Carbon Projection, 11, 2022

Ambitious Goal for GHG Emission Reduction

Achieving a 1.5°C planet will require the fastest economic transition in history, but the journey has already begun…

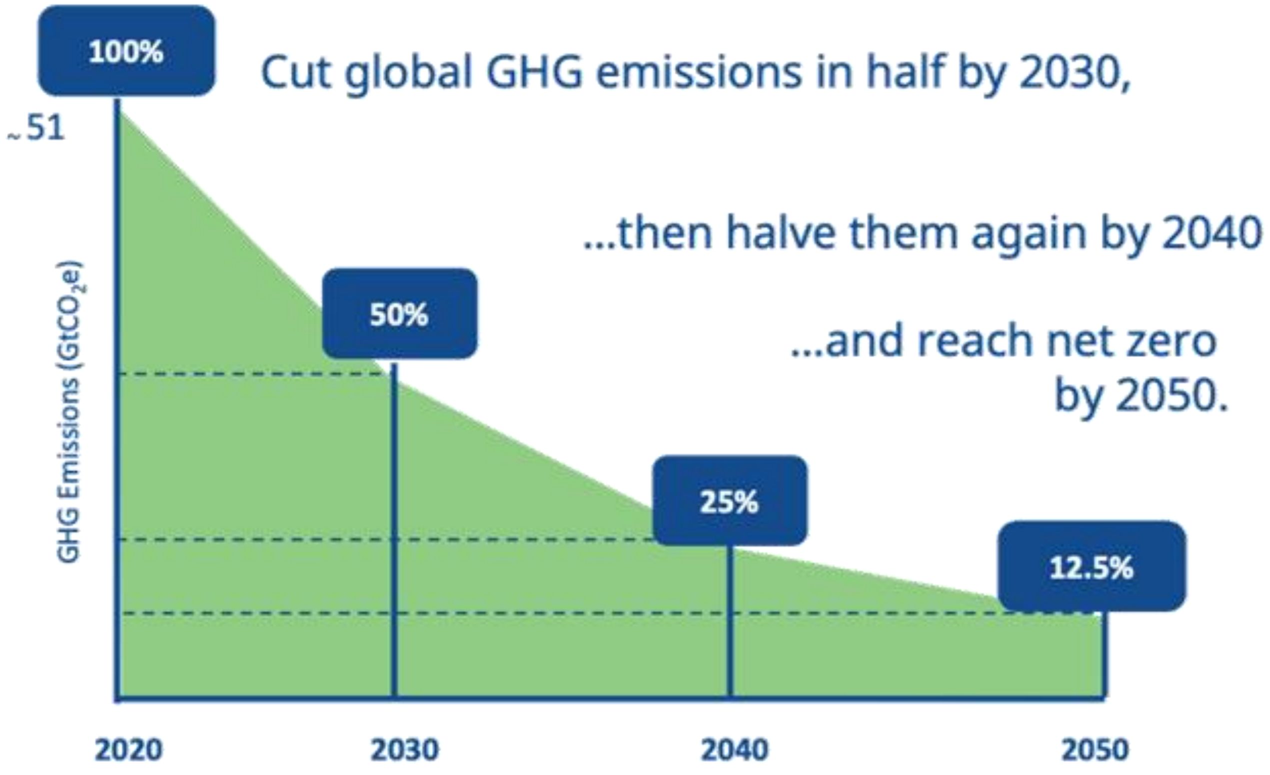
From Mike Train's talk on Emerson Sustainability

THE WORLD HAS A GOAL

The Paris Agreement sets out a global framework to avoid dangerous climate change by limiting global warming to **well below 2°C and pursuing efforts to limit it to 1.5°C.**

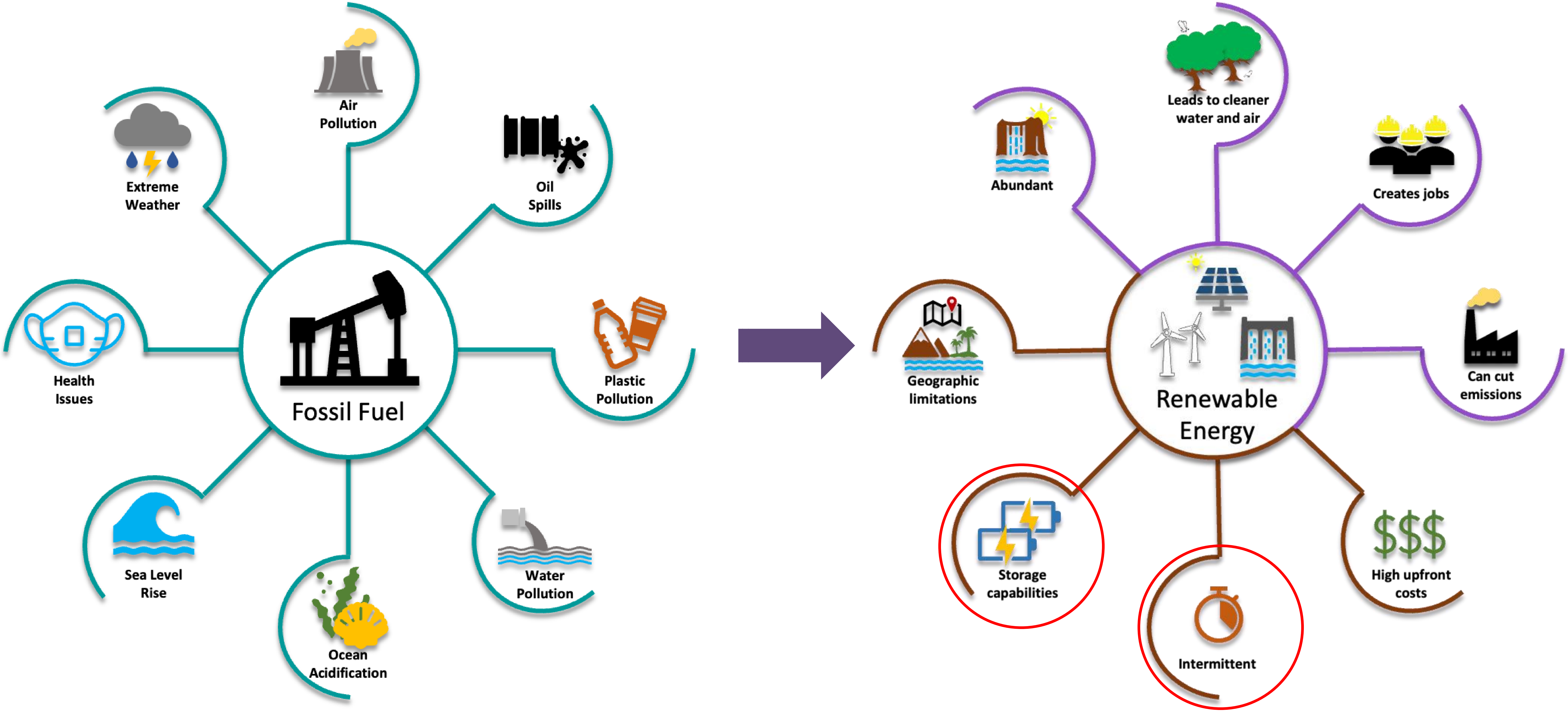
For this happen, the world must aim to:

The World Must Halve Emissions Every Decade

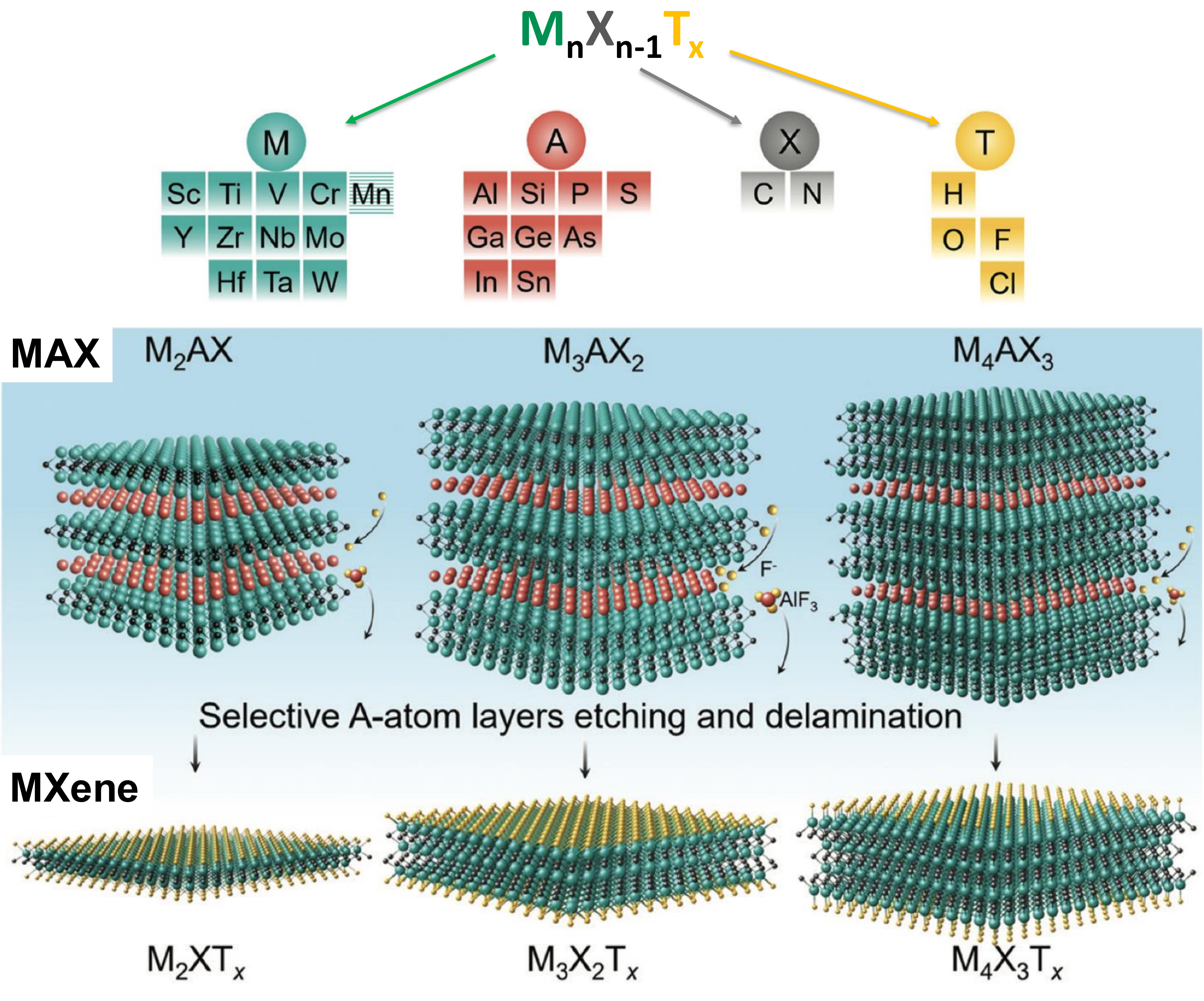


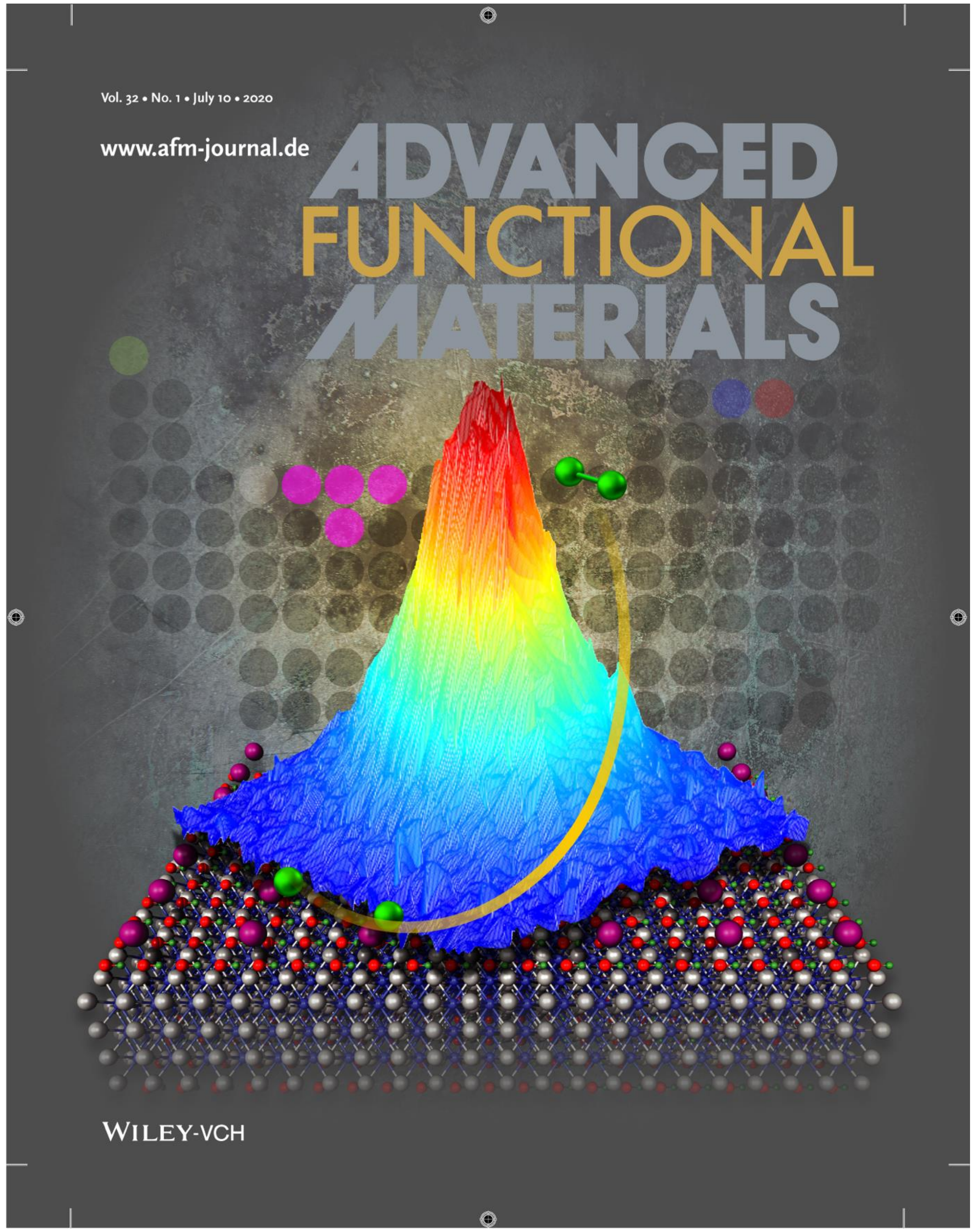
Adapted from EXPONENTIAL ROADMAP 1.5

Energy Transition is Needed



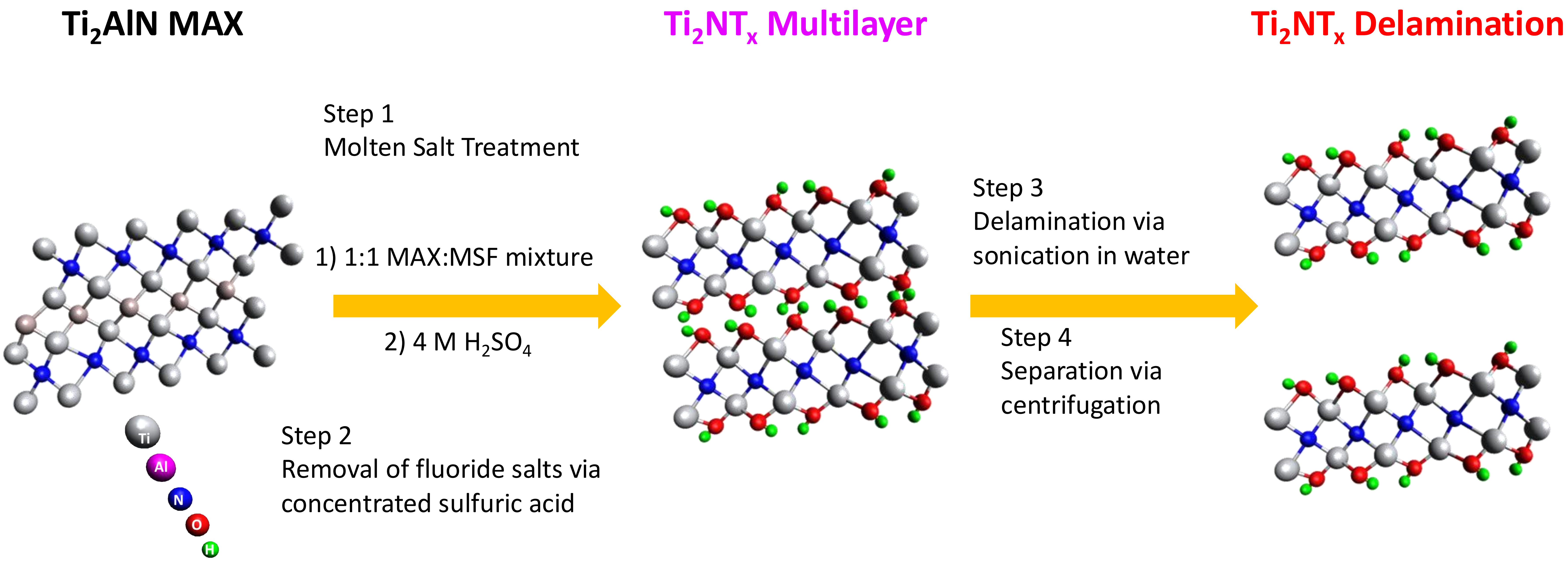
Emerging 2D Carbide & Nitride MXenes





Djire, A. et al. Adv. Funct. Matter, 2020, 18, 2001136

MNenes Synthesis via O_2-Assisted Molten Salt Fluoride

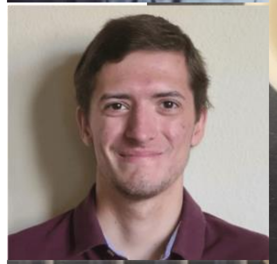


Johnson, D., Djire, A., et al. Scientific Reports, 2022, 12, 657

MNenes Synthesis via O_2-Assisted Molten Salt Fluoride

Bright Ugochukwu

Denis Johnson



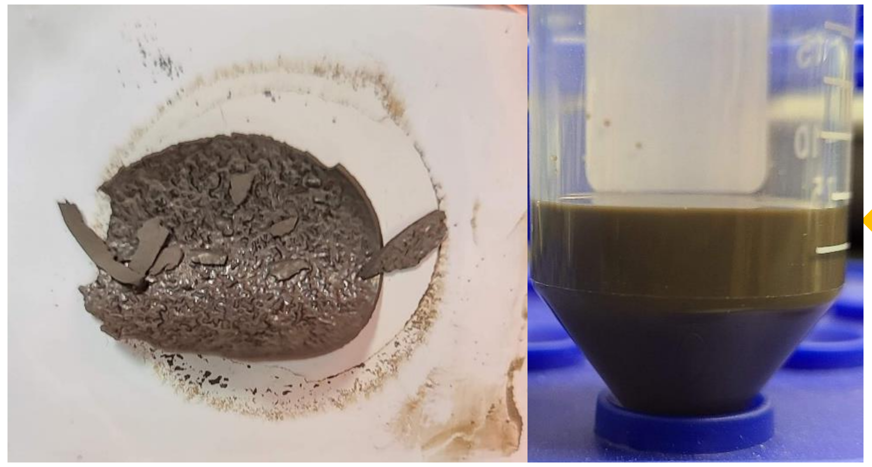
James Kasten

1) Ramp to 550 °C at 10 °C/min under Ar
2) Hold for 2 ½ hour under Ar; seal furnace
3) Hold for 2 ½ hour at 550 °C
4) Cool and hold at 450 °C
5) Quench to RT

1) Washing in 4 M Acid
2) Membrane Filter
3) Dry in Vacuum Oven

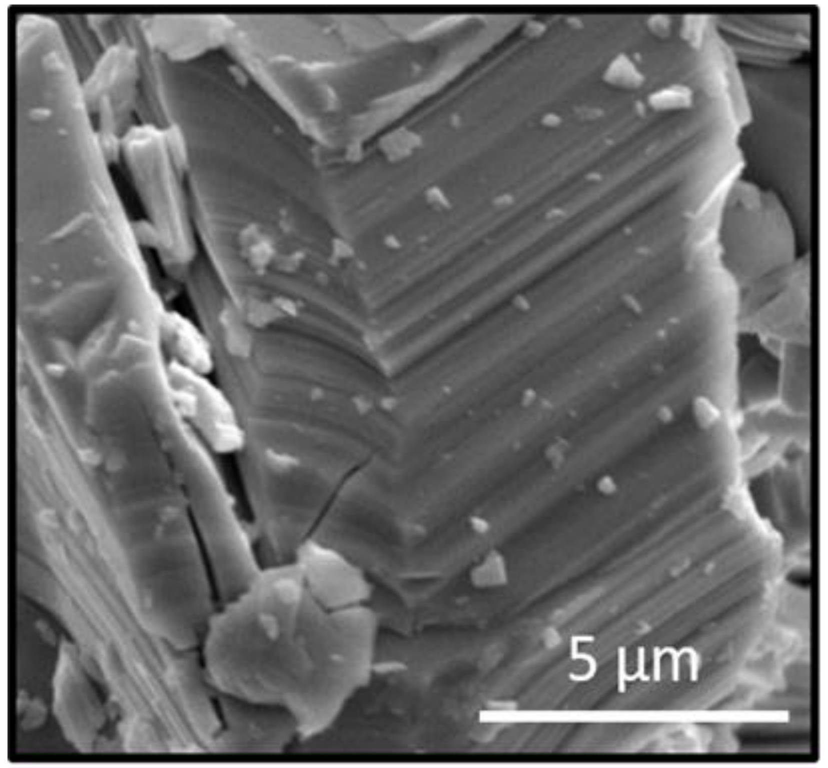
1) Disperse in water
2) Sonicate for 30 minutes
3) Let Rest for 2 hours
4) Membrane filter

Few to Single Layer MXene

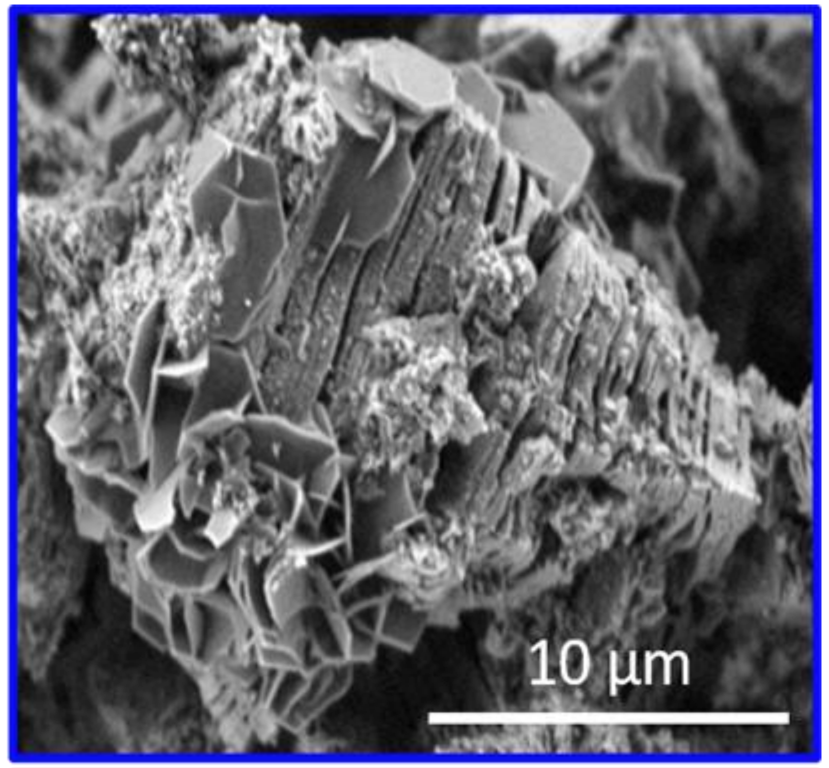


MAX to MNenes Morphology

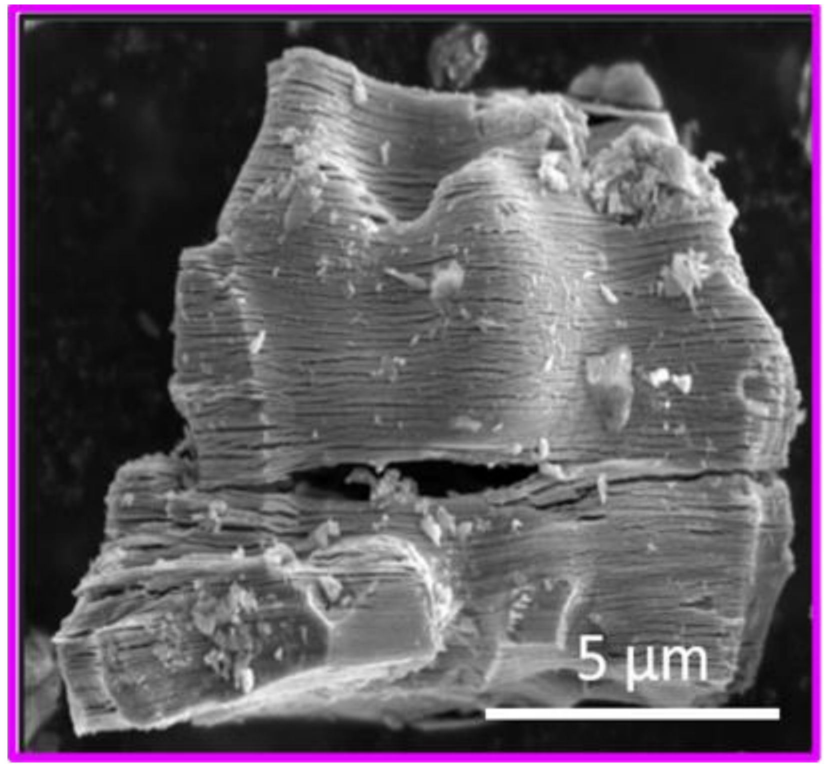
Ti_2AlN MAX Phase

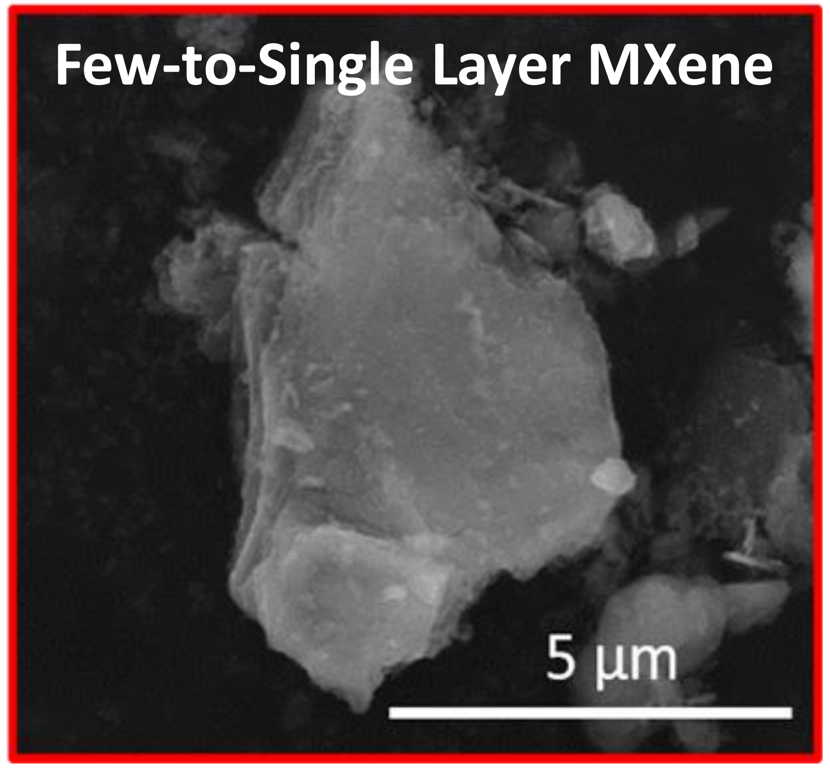


Molten Salt Treated MAX



Multilayer Ti_2N MXene

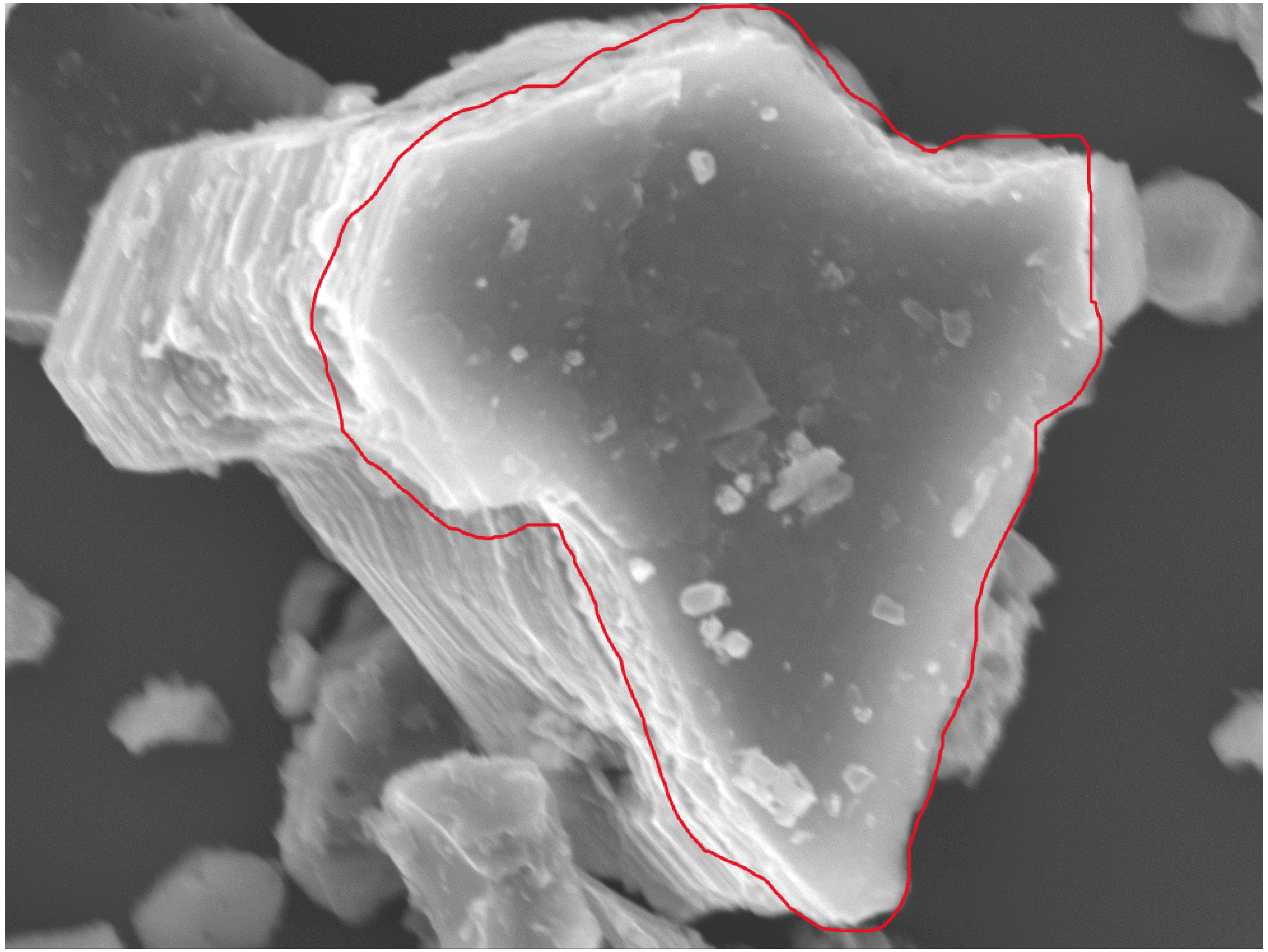




Johnson, D., Djire, A., et al. Scientific Reports, 2022, 12, 657

Africa in 2D MNene!

Image collected by
Bright Ugochukwu



Ngozichukwu, B., Djire, A., et al. ACS Appl. Nano Mater., 2024, 7, 11, 13765–13774

Africa in 2D MNene!

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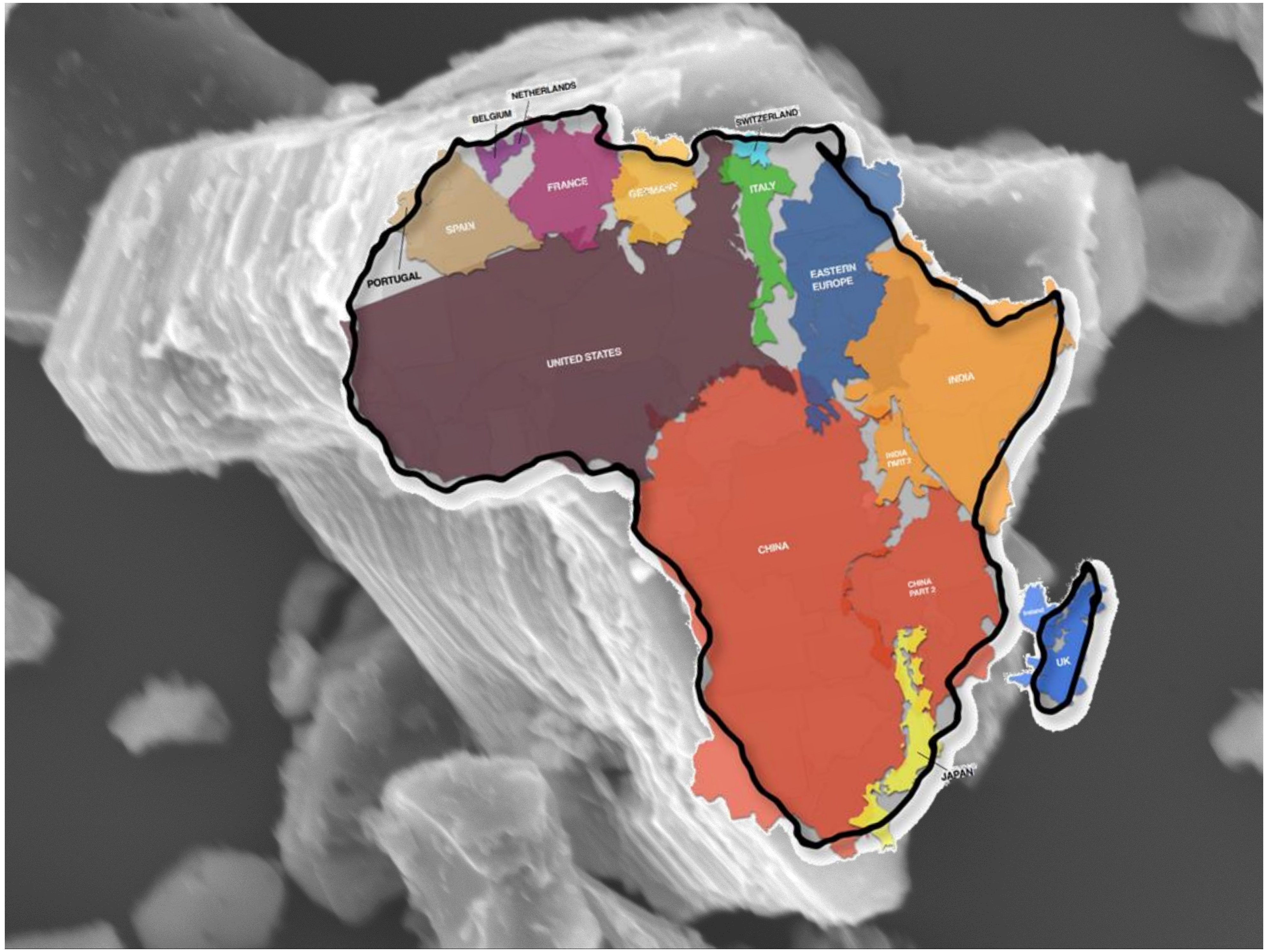
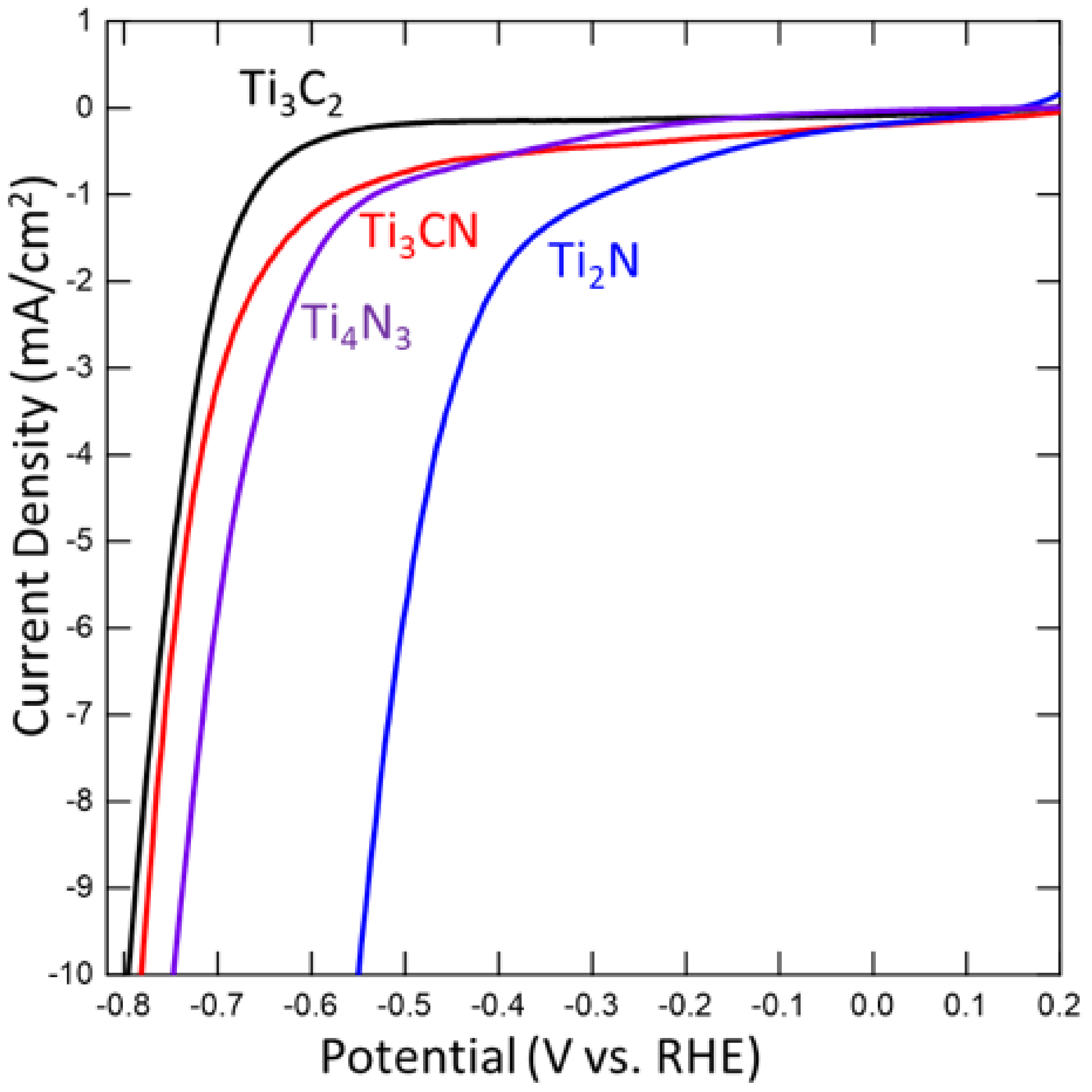
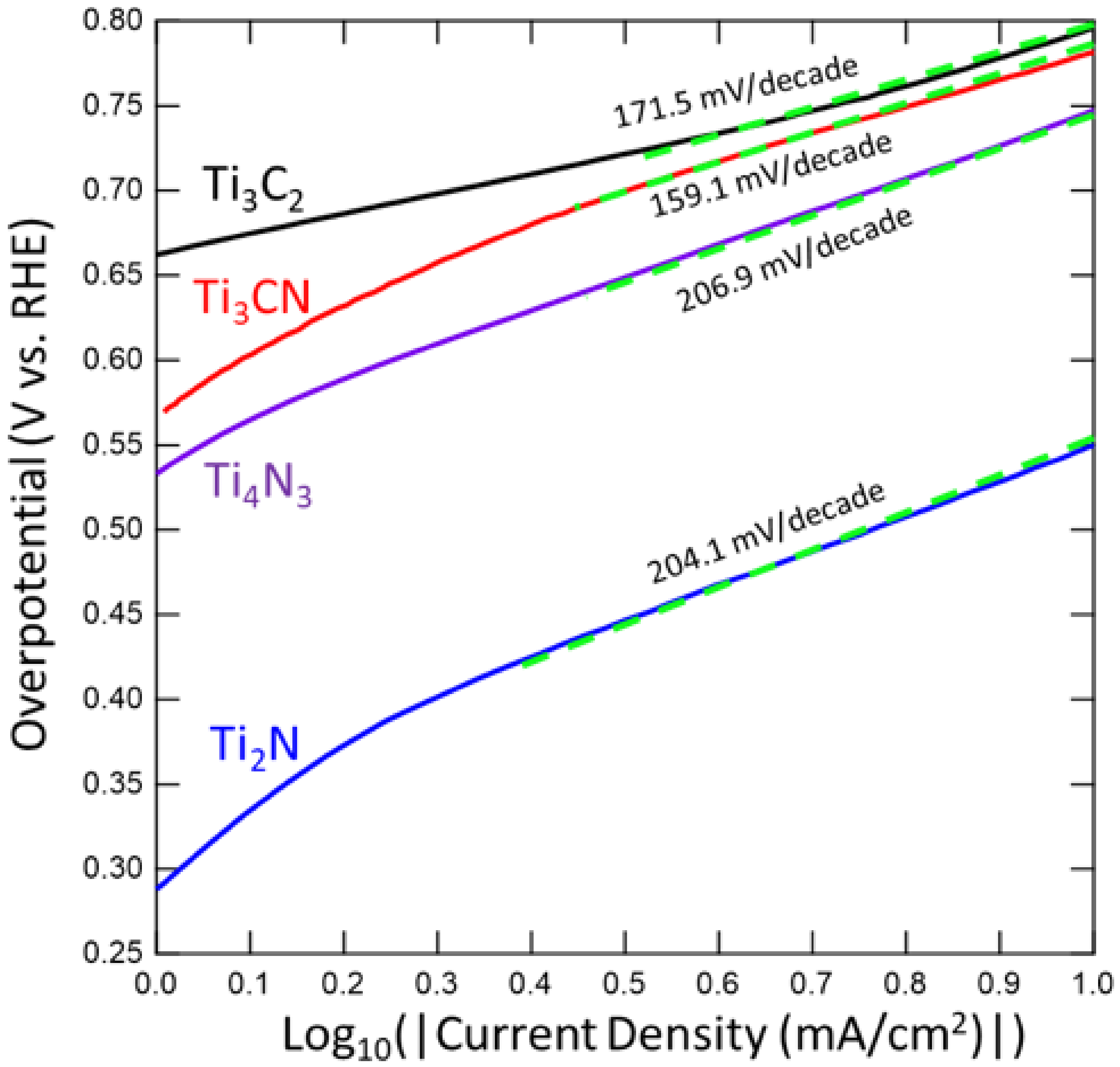


Ngozichukwu, B., Djire, A., et al. ACS Appl. Nano Mater., 2024, 7, 11, 13765–13774

Electrocatalytic Behavior of MNenes in Acidic Media

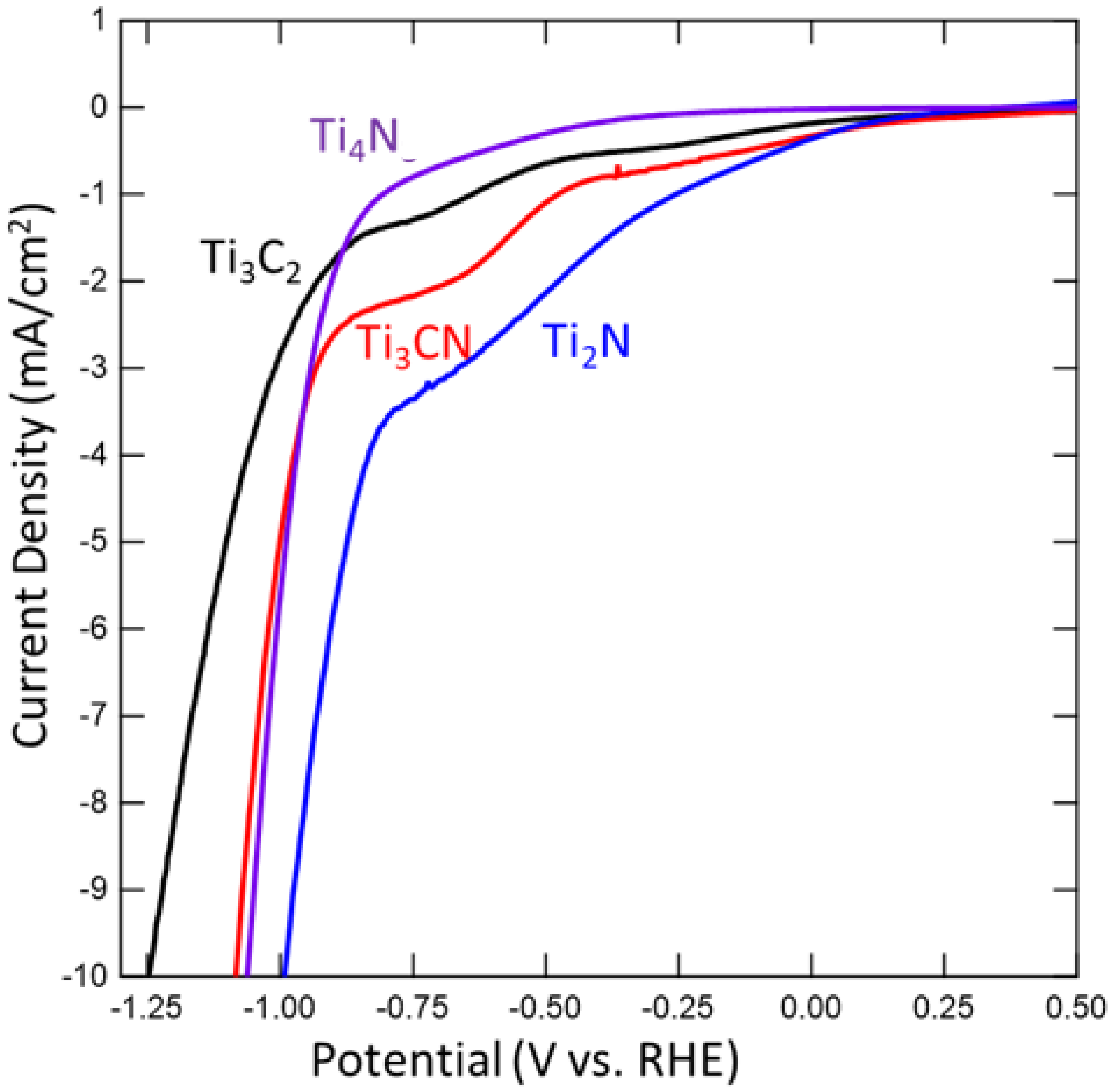


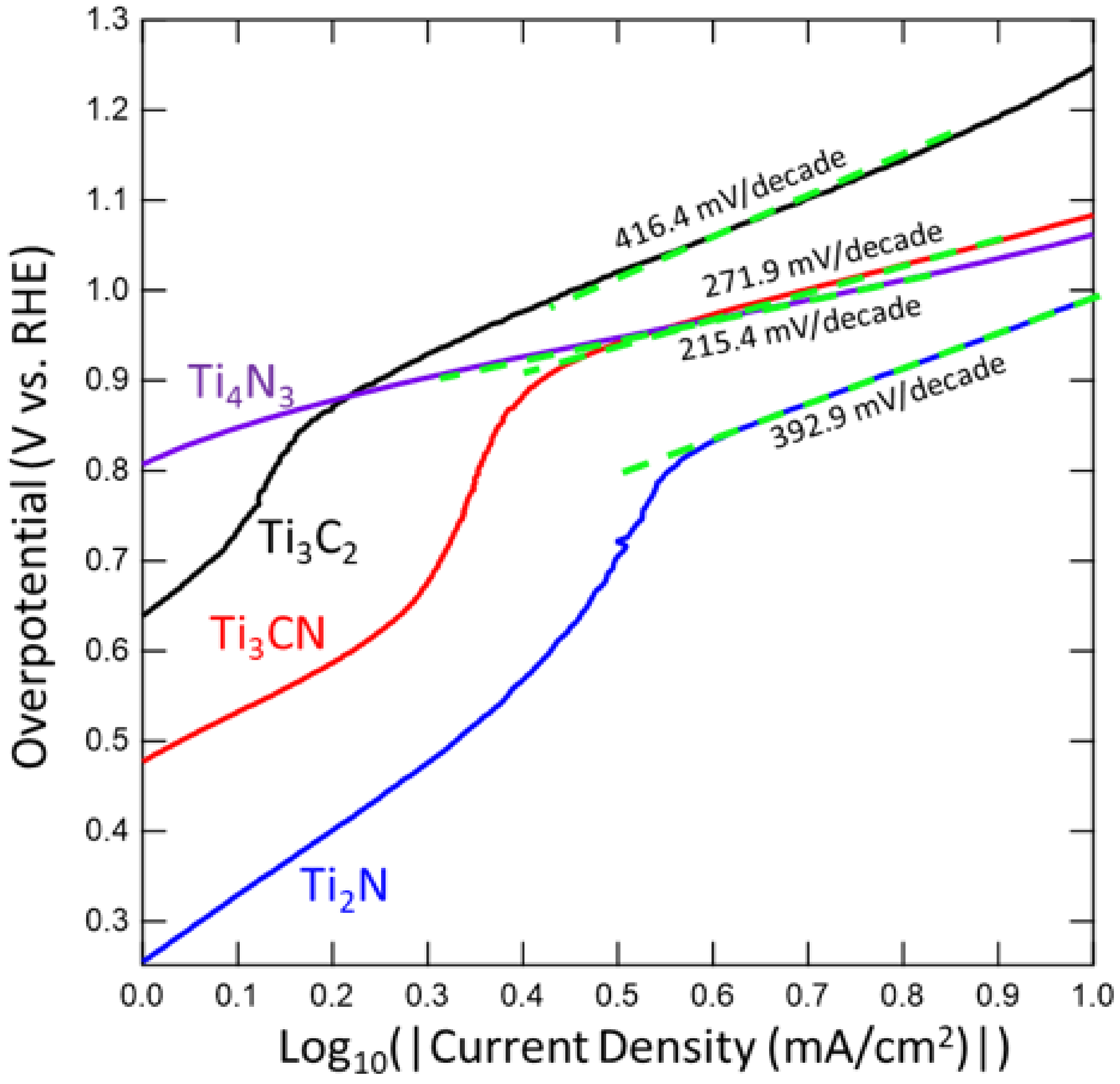


Electrolyte: 0.5 M HCl

MXene candidates are not good for HER

Electrocatalytic Behavior of MNenes in Neutral Media

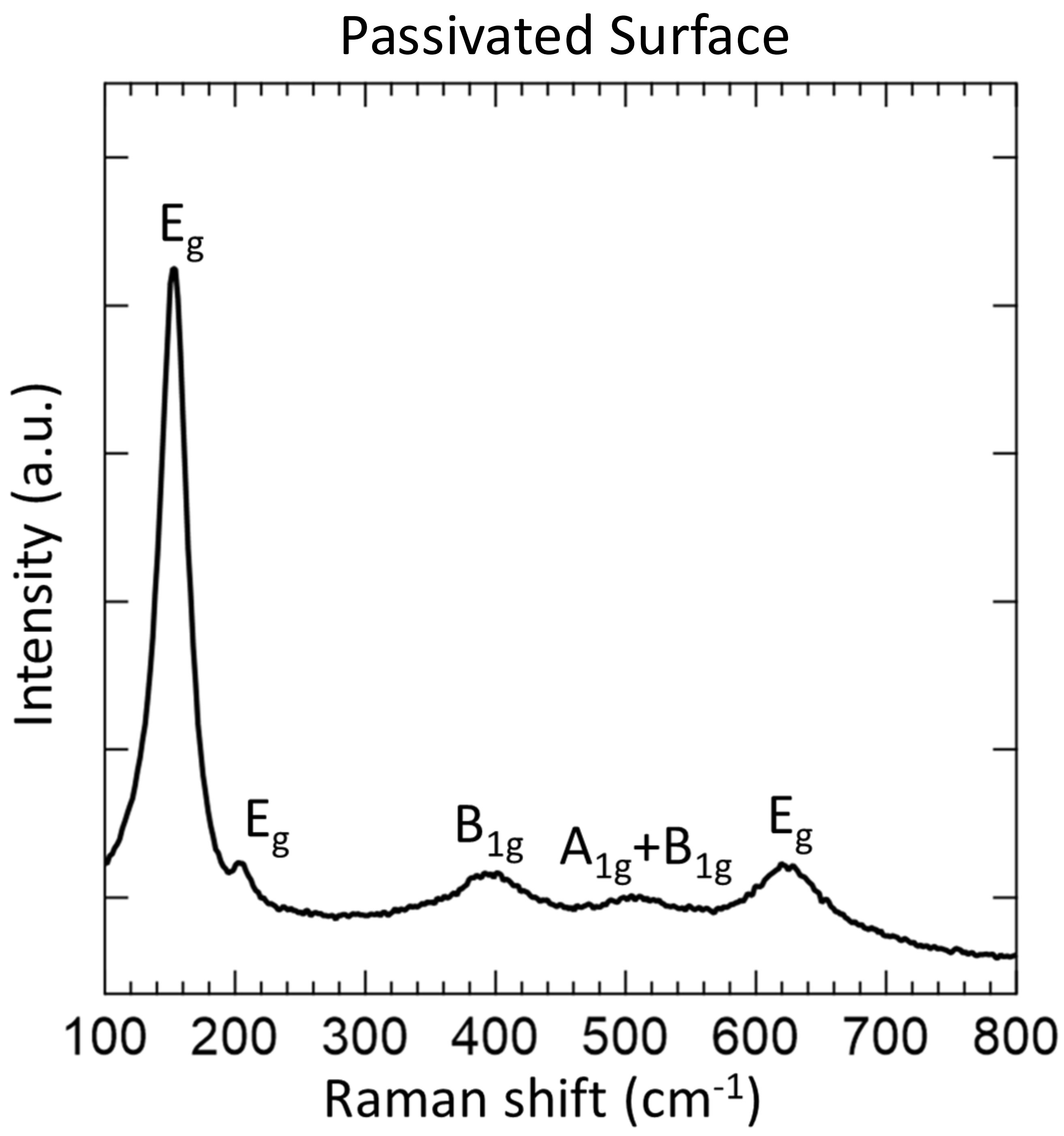


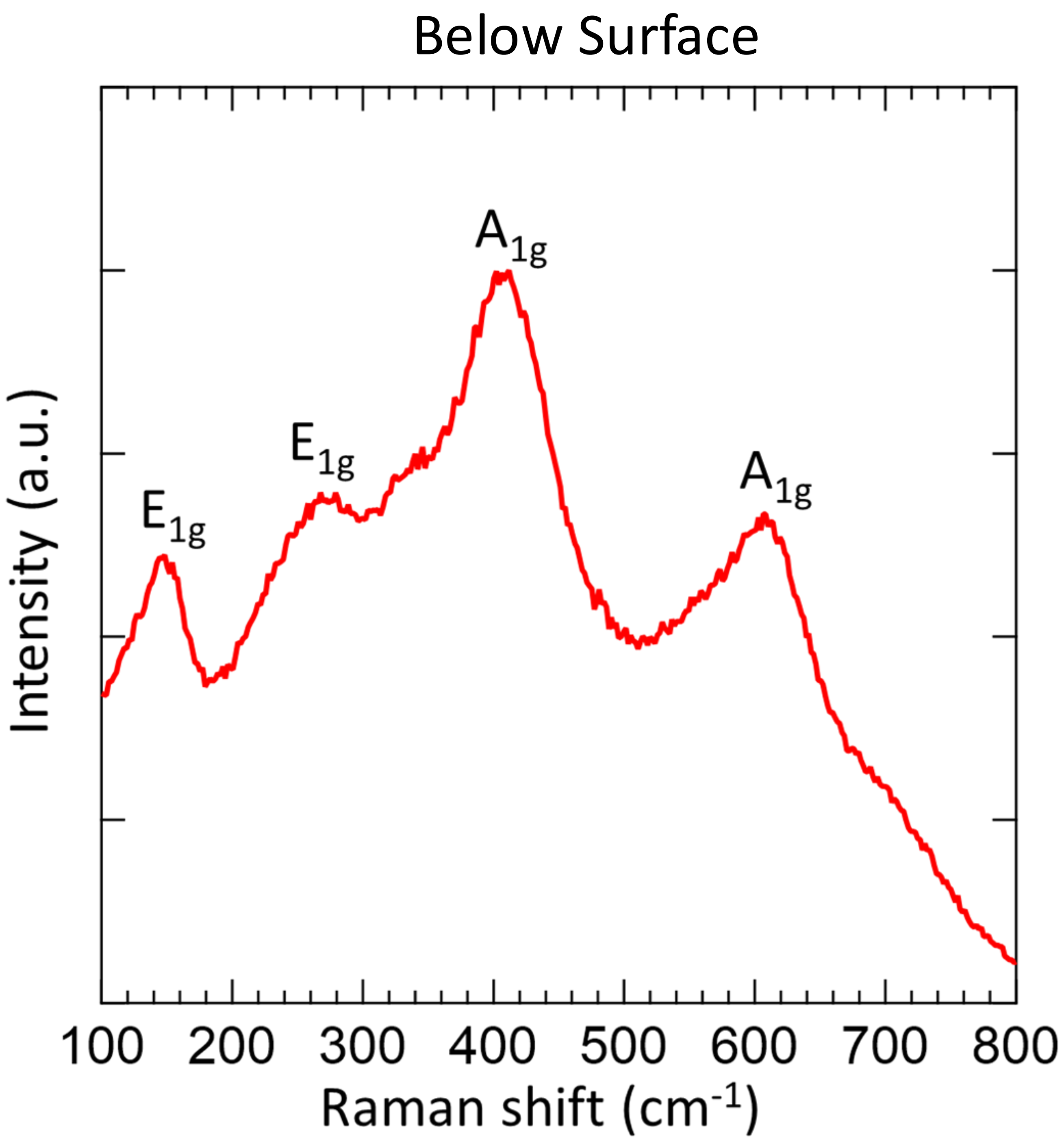


Electrolyte: 0.5 M Na_2SO_4

MXene candidates are not good for HER

Pristine Ti_2NT_x with Passivation Layer

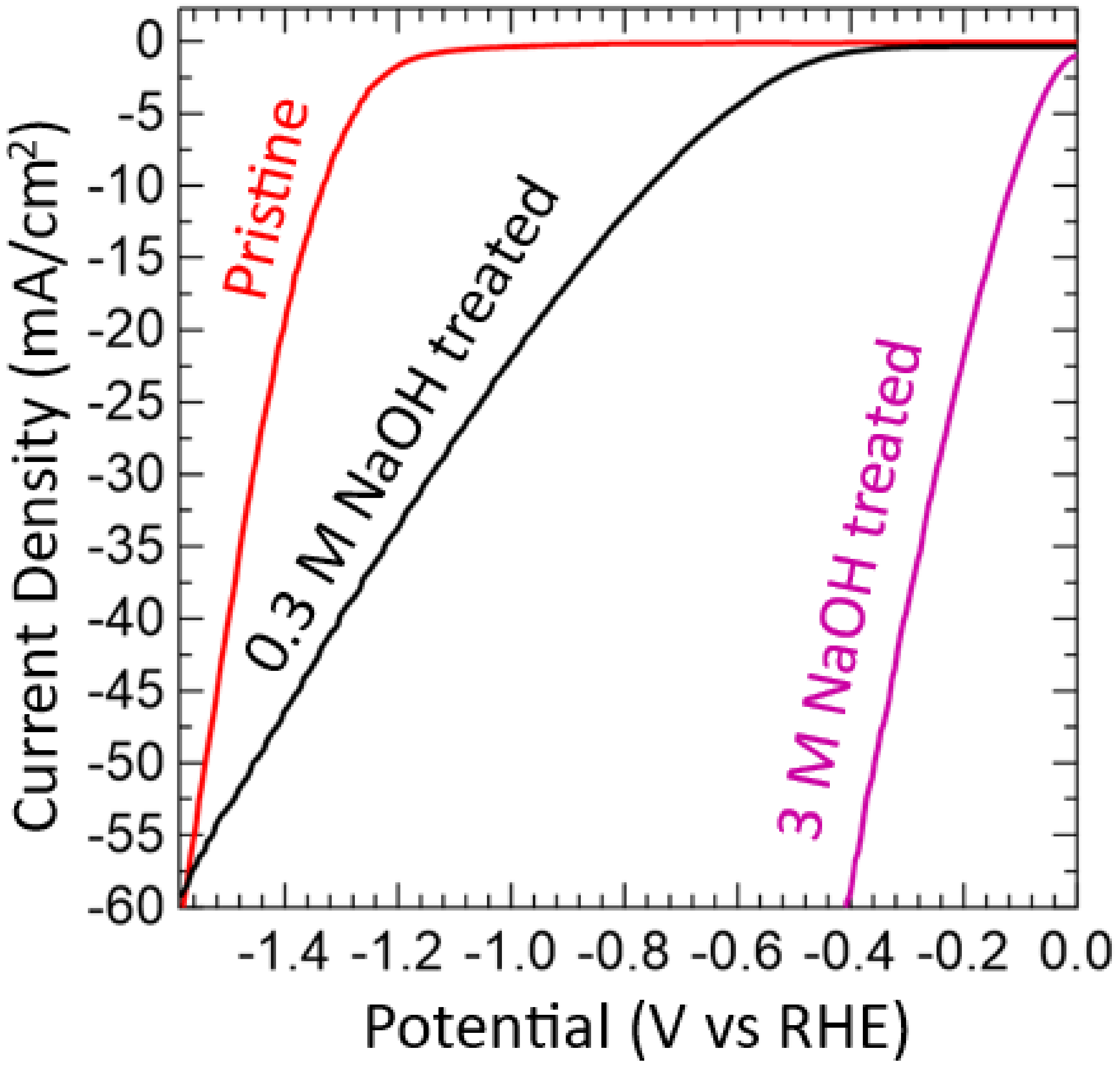


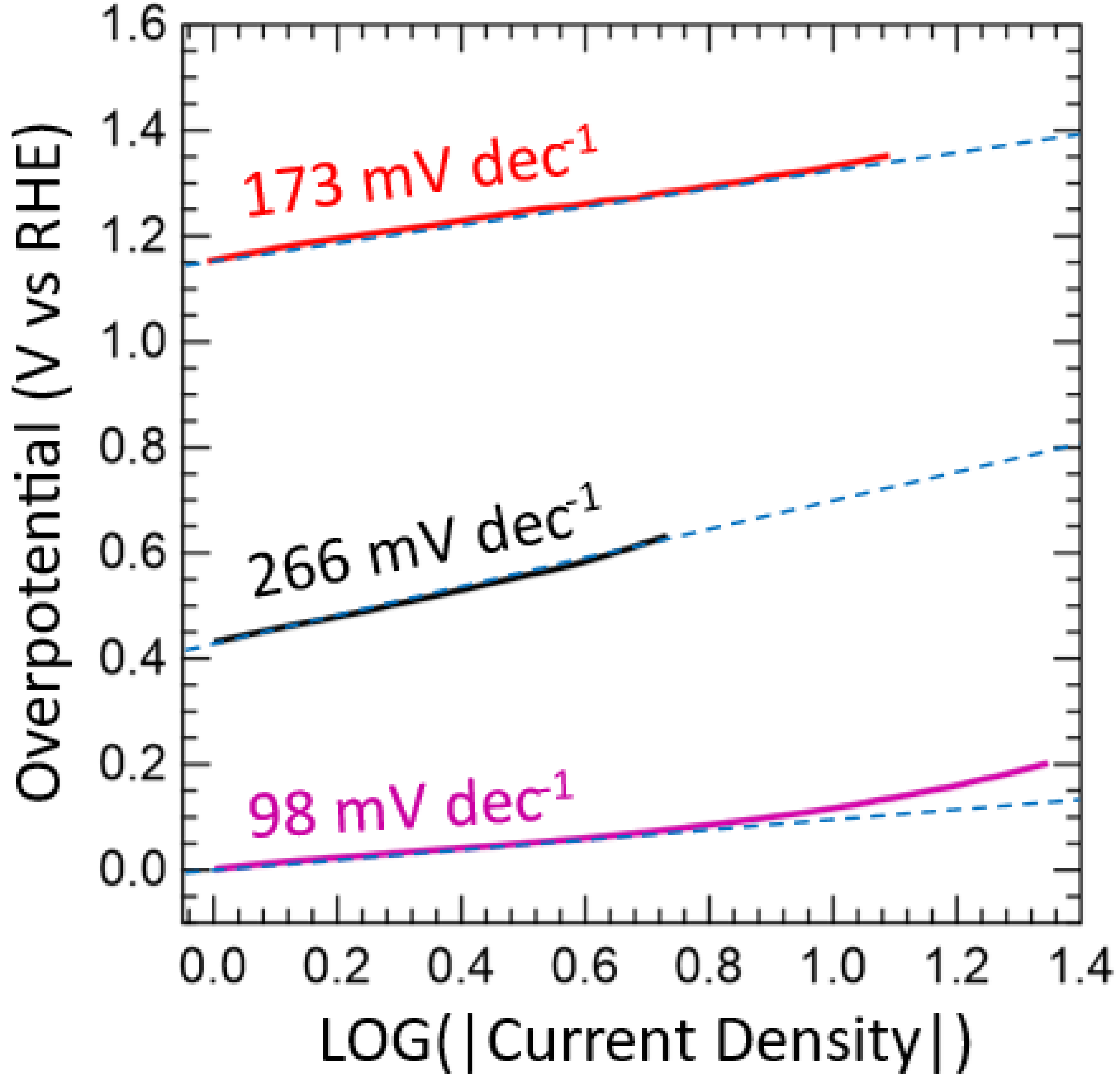


Passivated surface protects MNene but renders basal plane inactive for HER

Yoo, R., and Djire, A. ACS Catalysis, 2023, 13, 6823-6836

Tuning Ti_2NT_x HER Activity in Alkaline Electrolytes



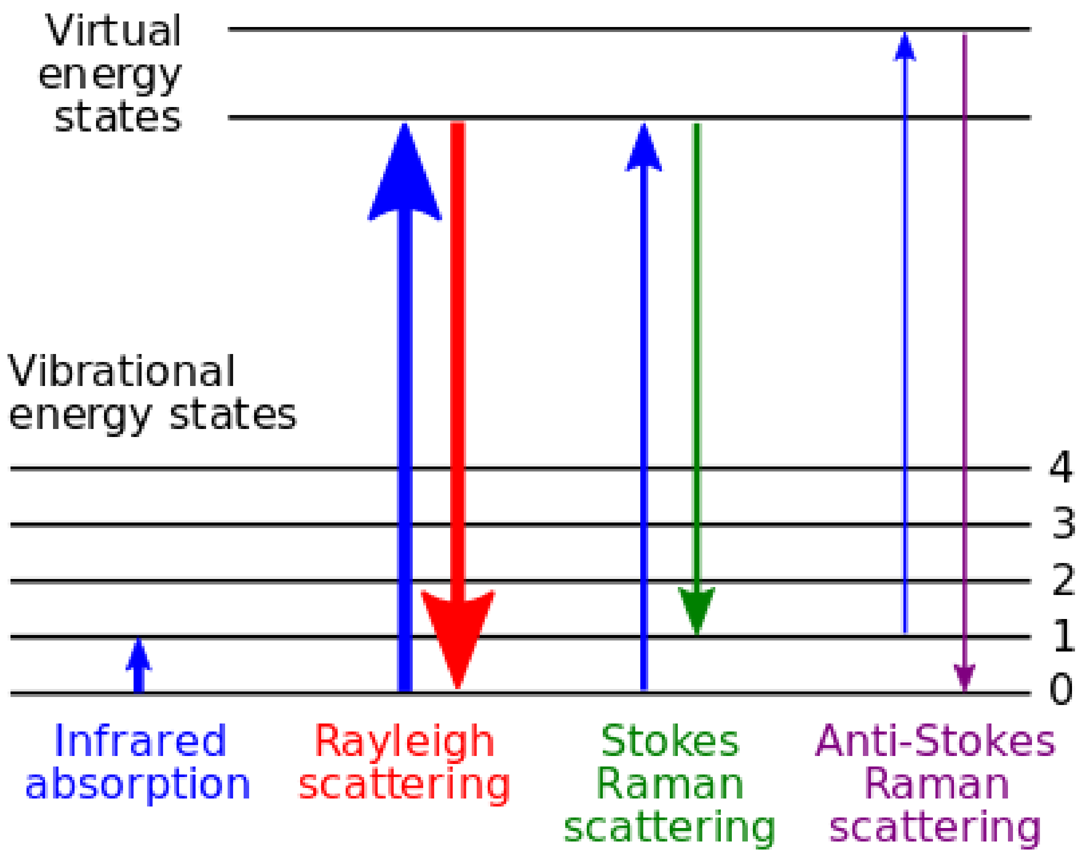


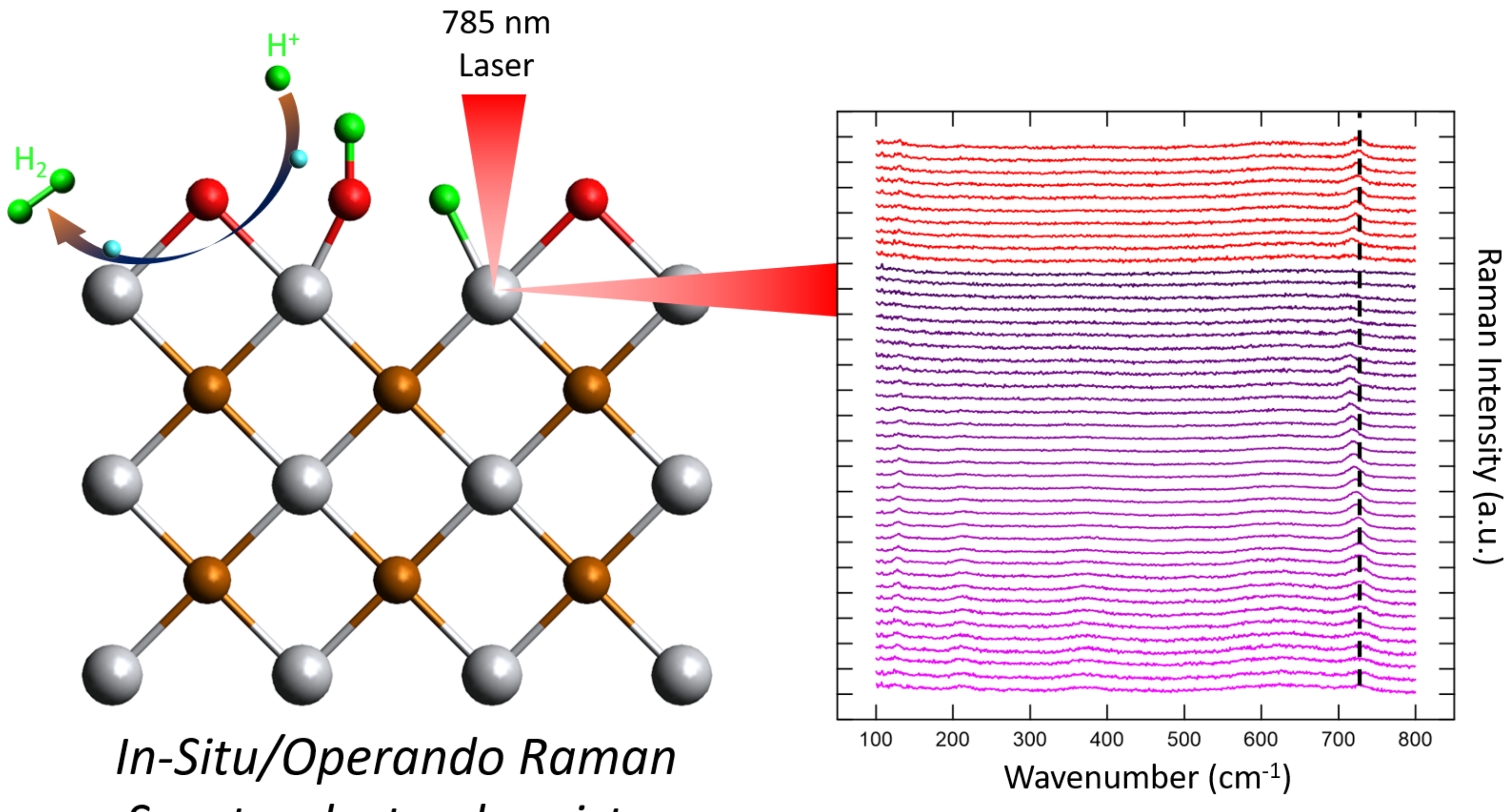
Ray Yoo

Removal of passivation layer enhances HER activity

Yoo, R., and Djire, A. ACS Catalysis, 2023, 13, 6823-6836

Insights Into the HER Mechanism





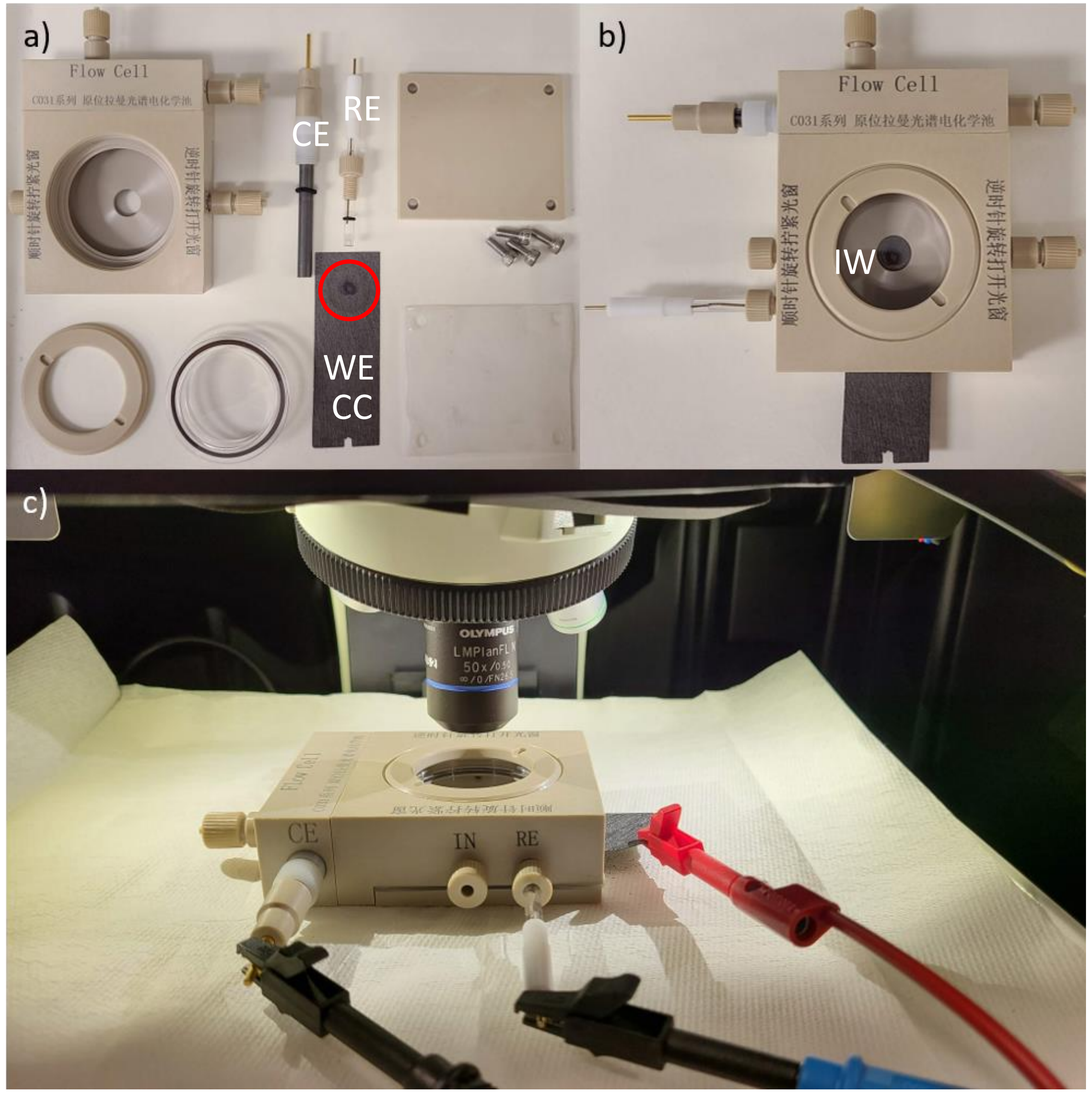
In-Situ/Operando Raman Spectroelectrochemistry

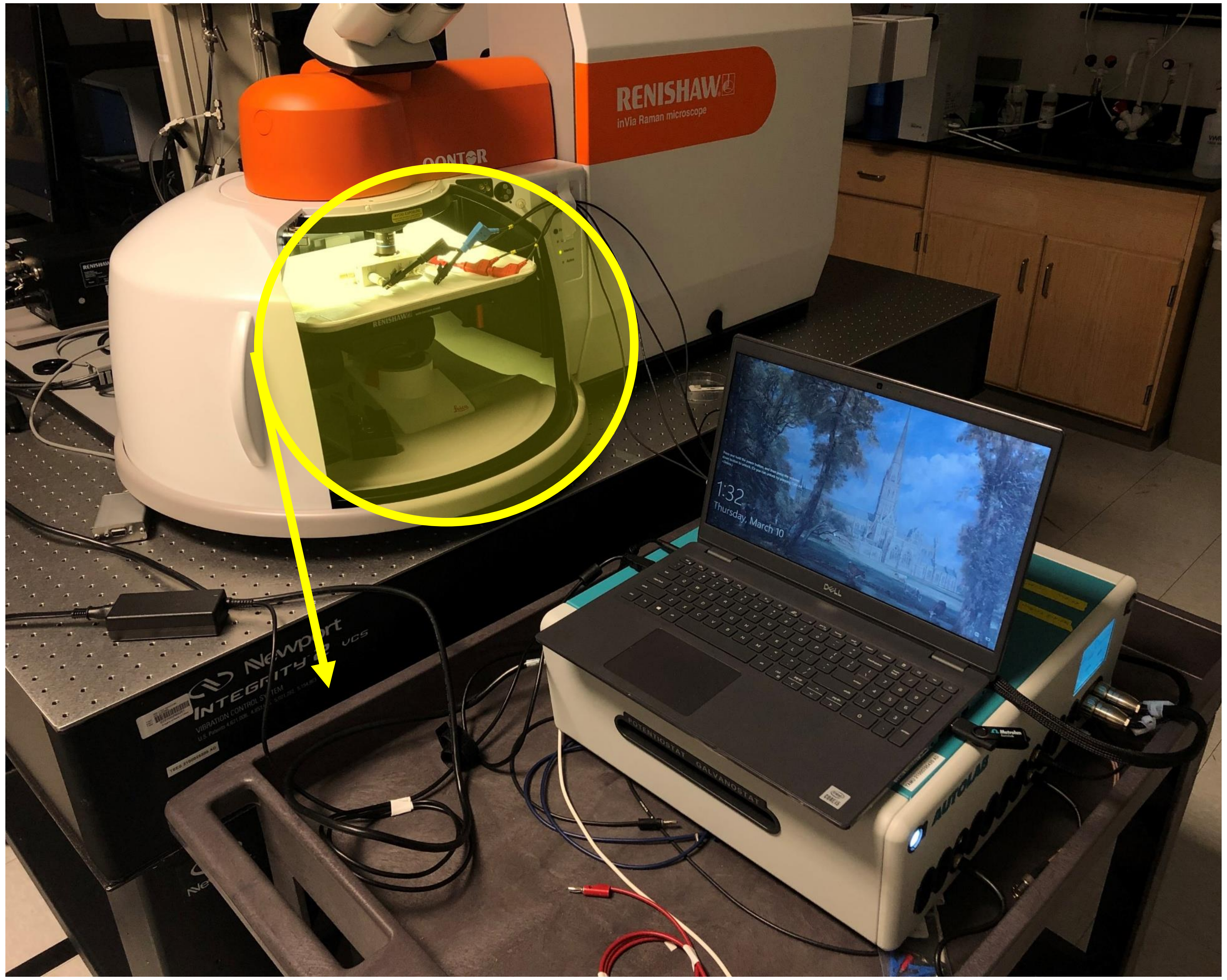
Why MXenes are not good for HER?
What makes them good for HER?

Kyle Hansen

Denis Johnson

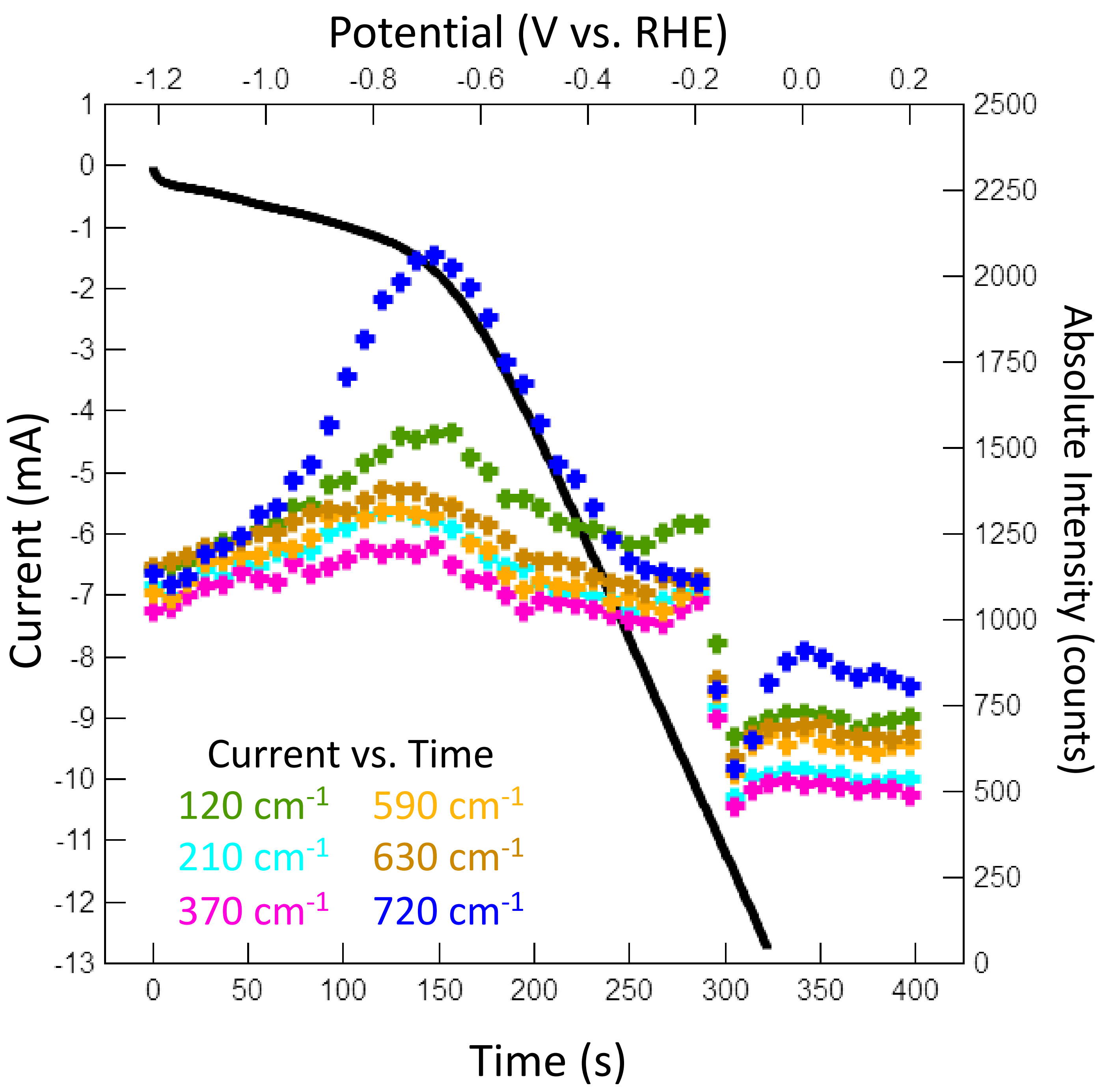
In-Situ/Operando Raman Spectroelectrochemistry



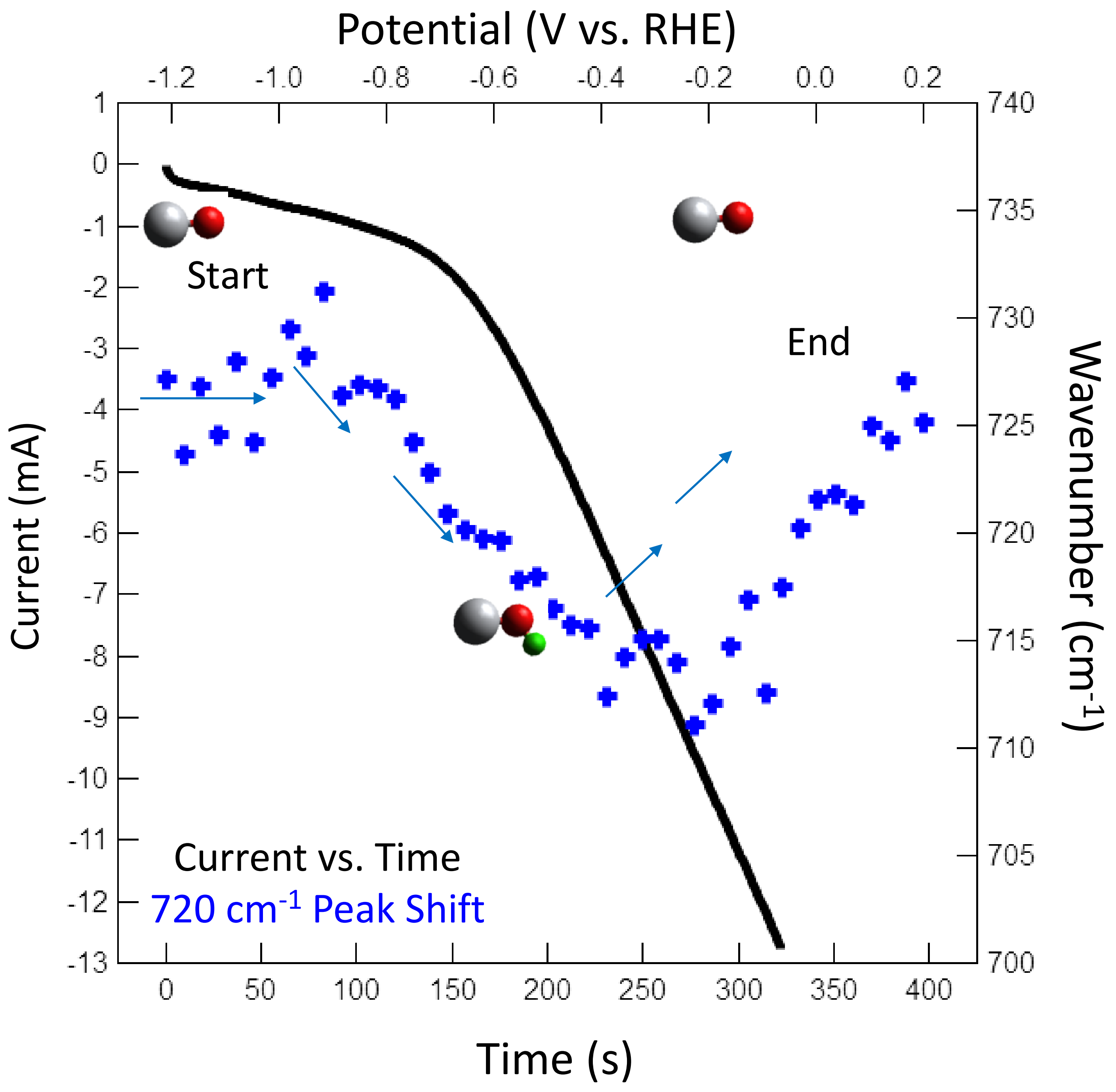


IW = Illumination window   CC = Current Collector   WE = Working Electrode   RE = Reference Electrode   CE = Counter Electrode

In-Situ Raman Spectroelectrochemistry in Acidic Media

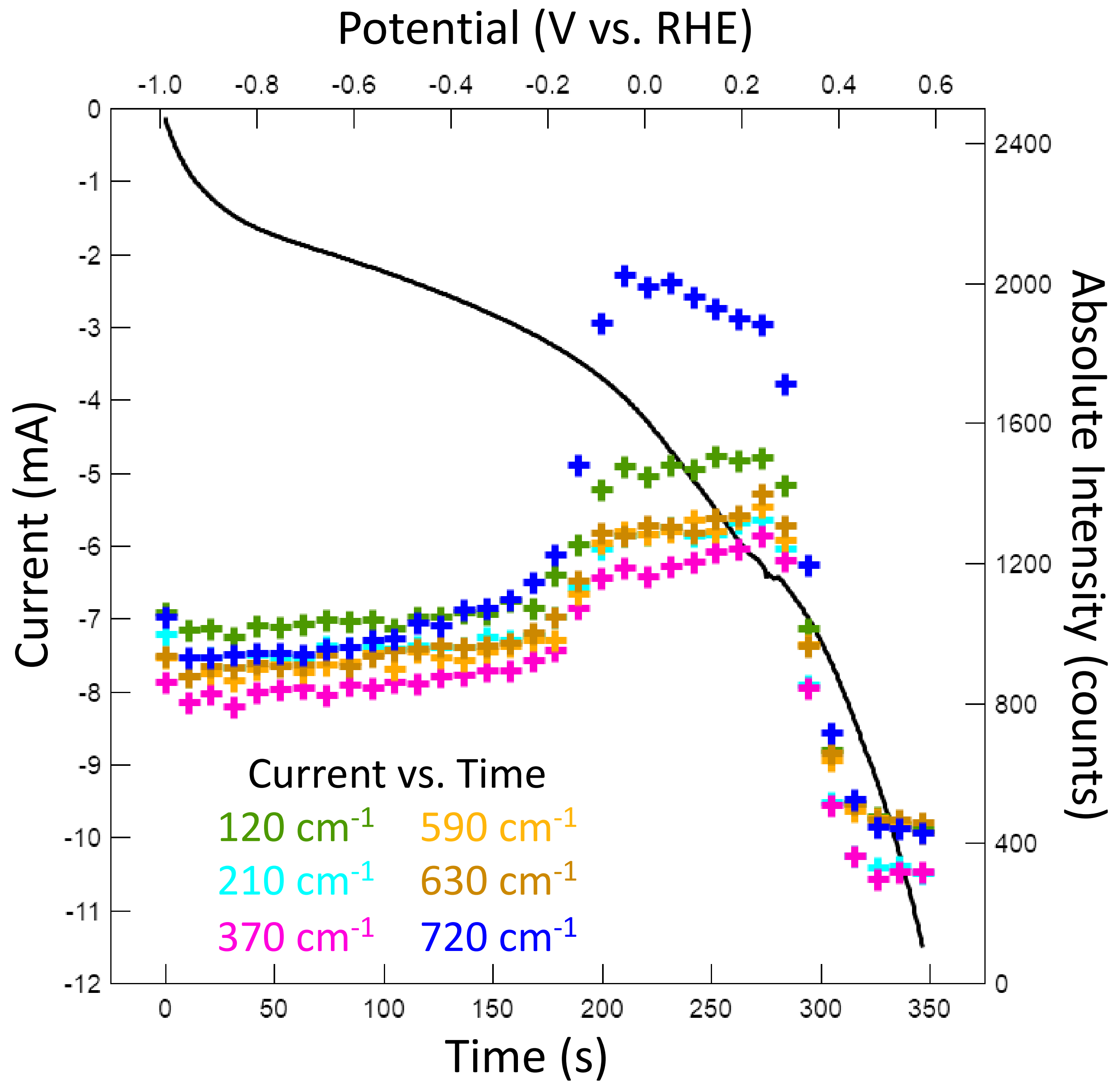


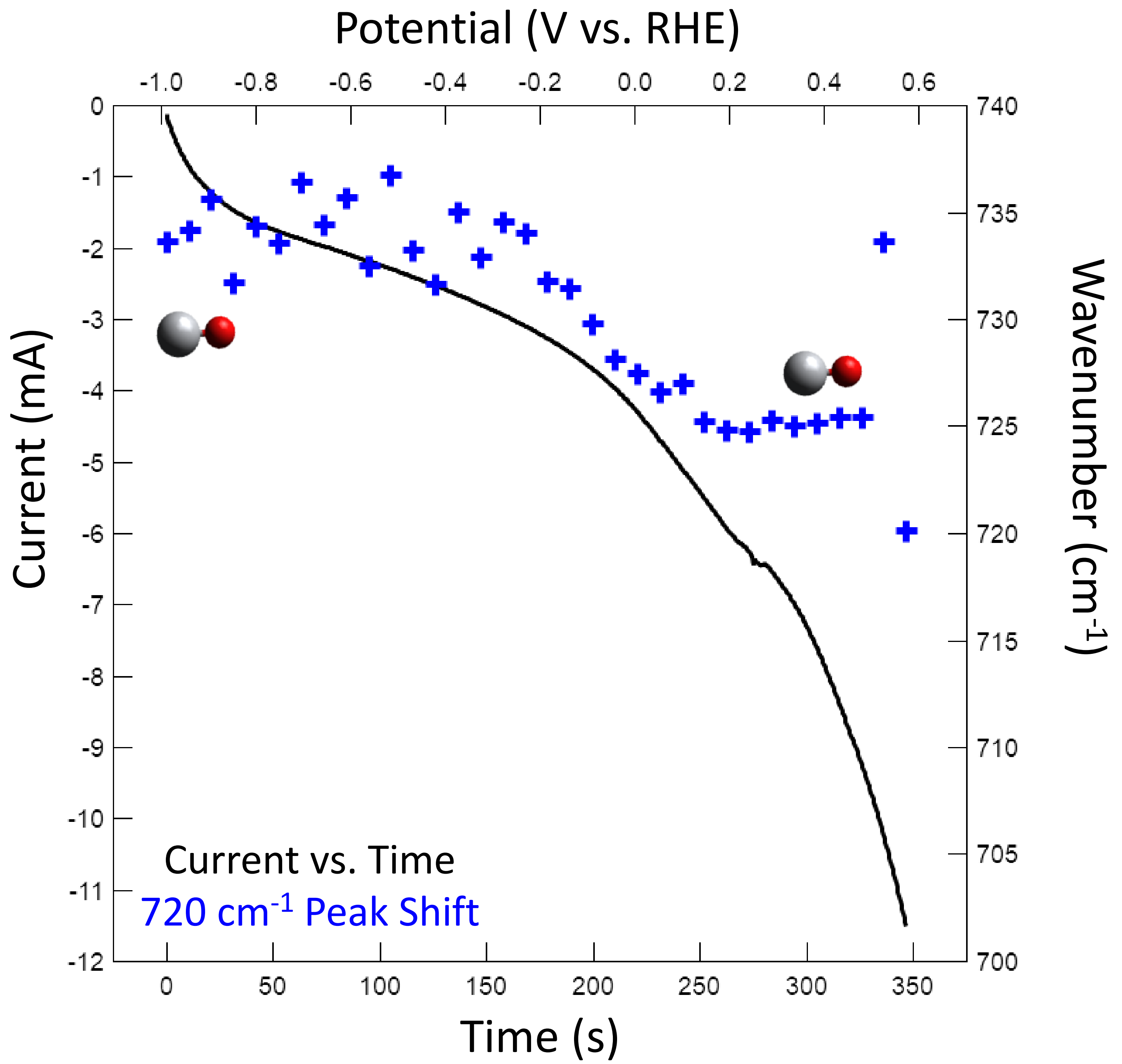
D. Johnson, A. Djire, et al., Nanoscale (2022)



0.1 M HCl electrolyte

In-Situ Raman Spectroelectrochemistry in Neutral Media

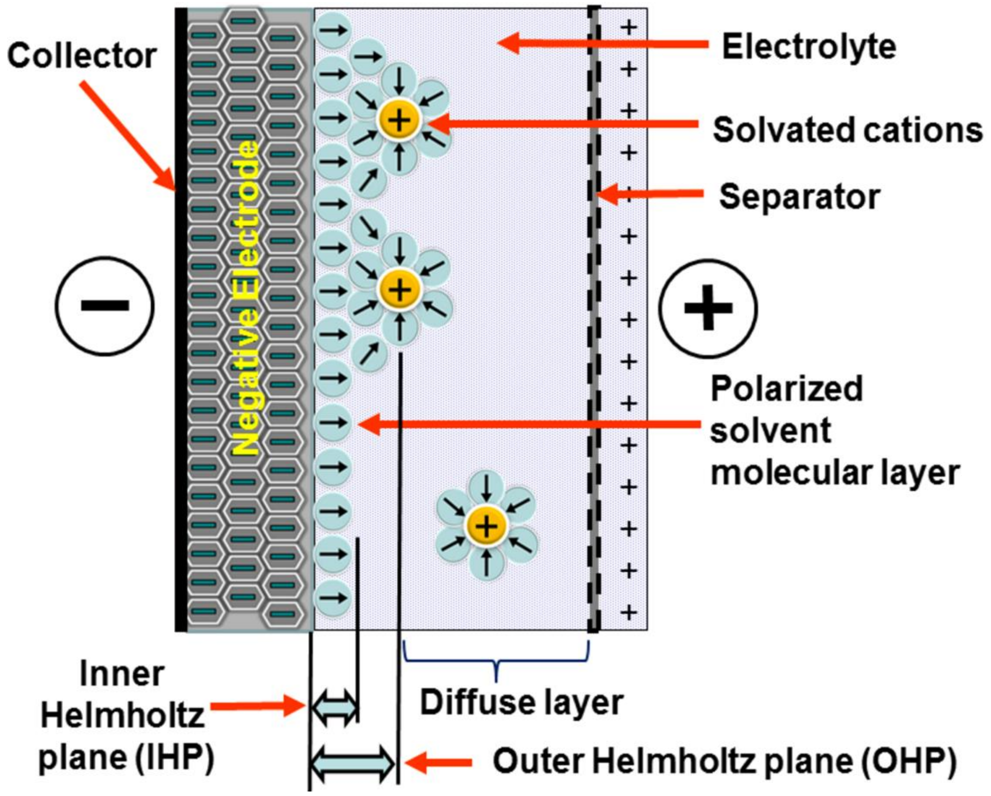




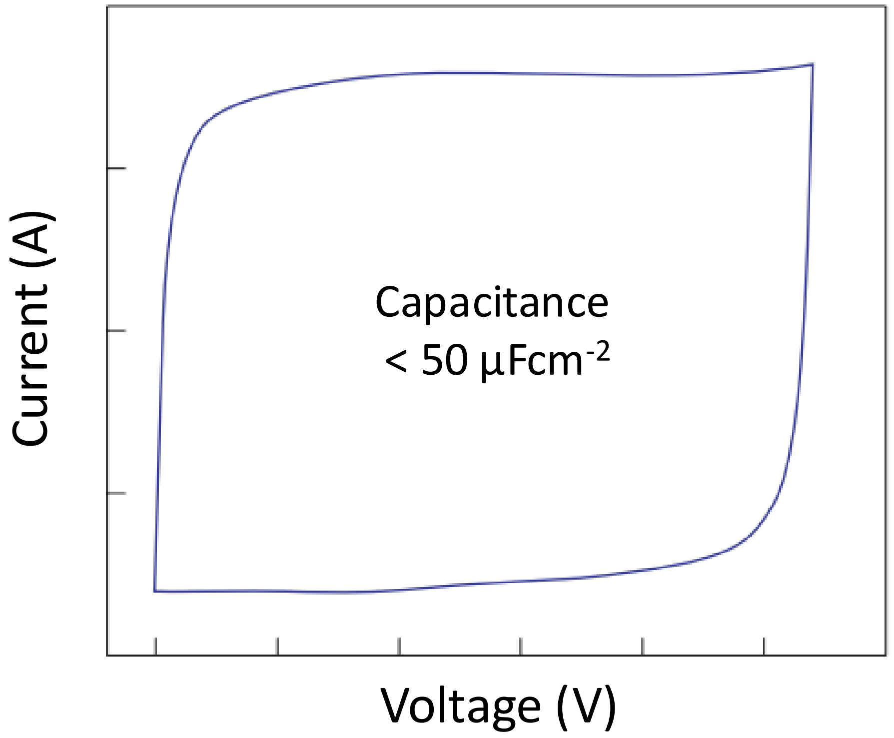
D. Johnson, A. Djire, et al., Nanoscale (2022)

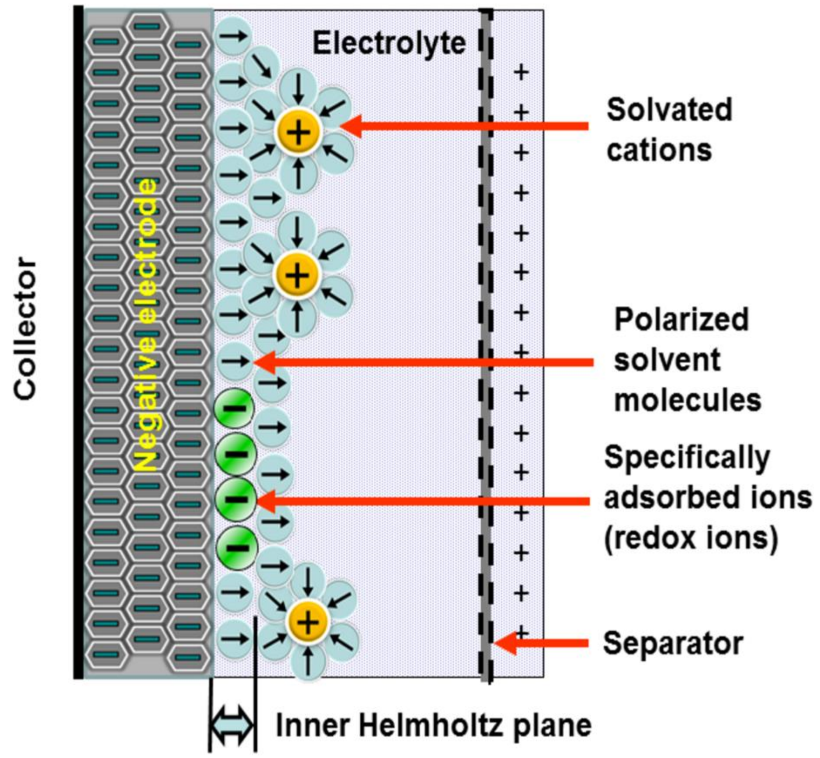
0.1 M Na_2SO_4 electrolyte

Double Layer vs. Pseudocapacitance

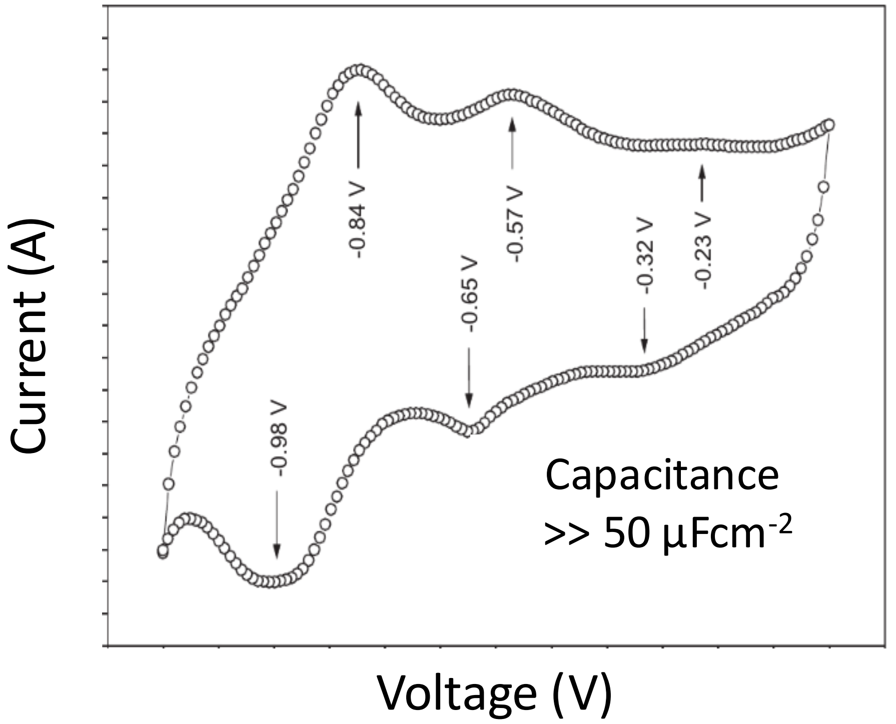


Double-layer capacitance



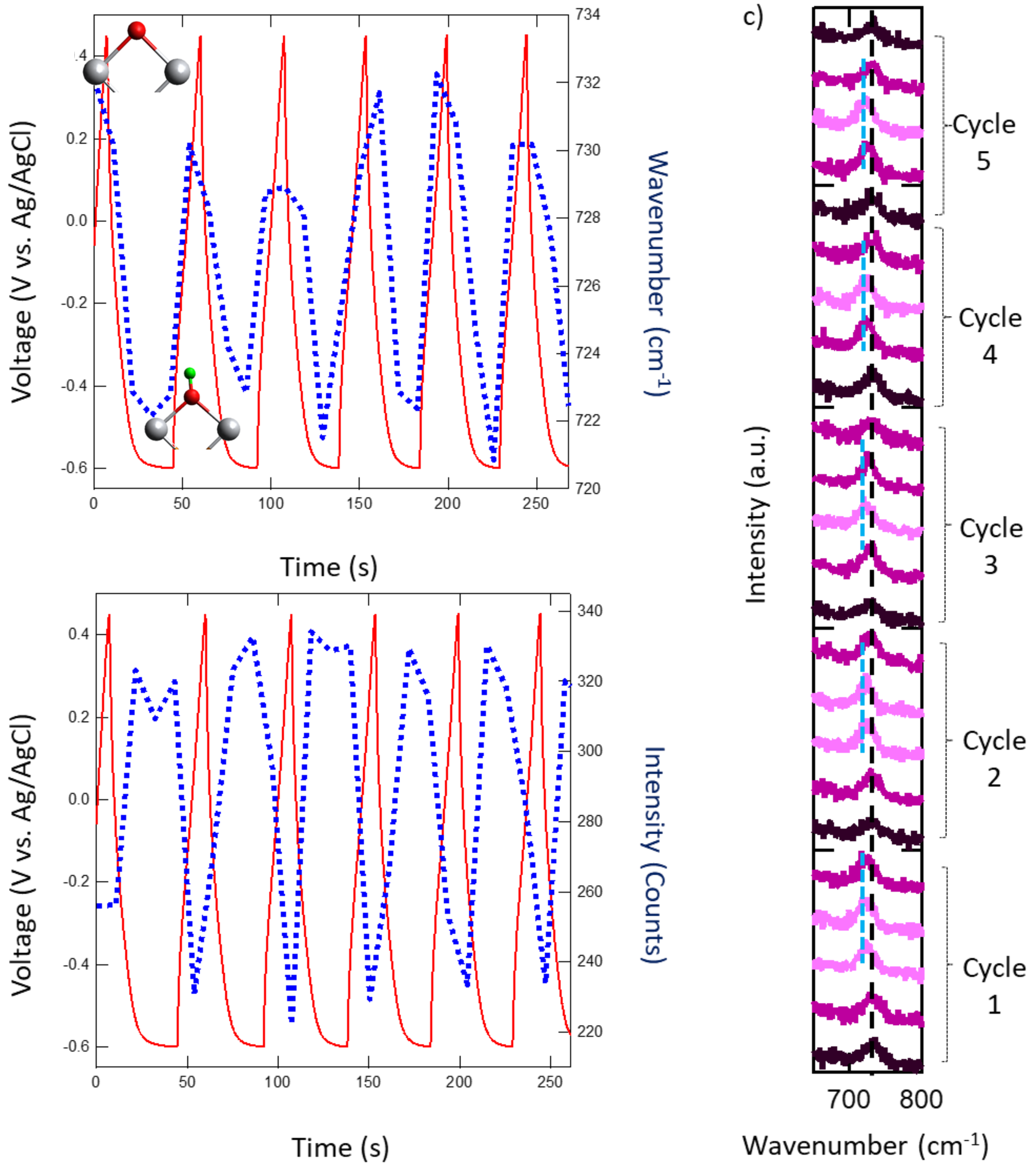


Pseudocapacitance

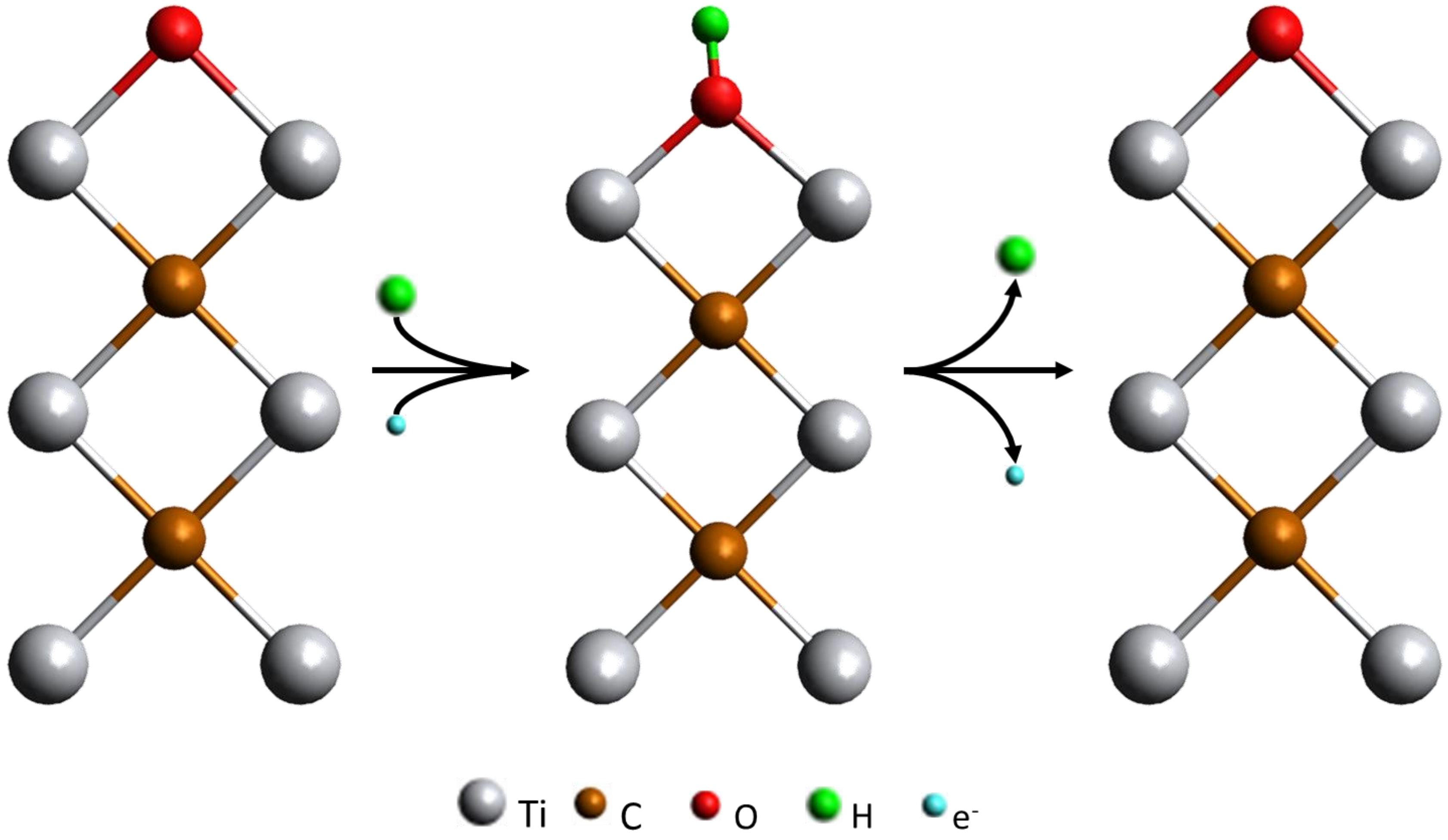


Charge Storage Principles of EDLC (2013)   Charge Storage in Pseudocapacitors (2013)

Energy Storage Mechanism in Acidic Electrolyte



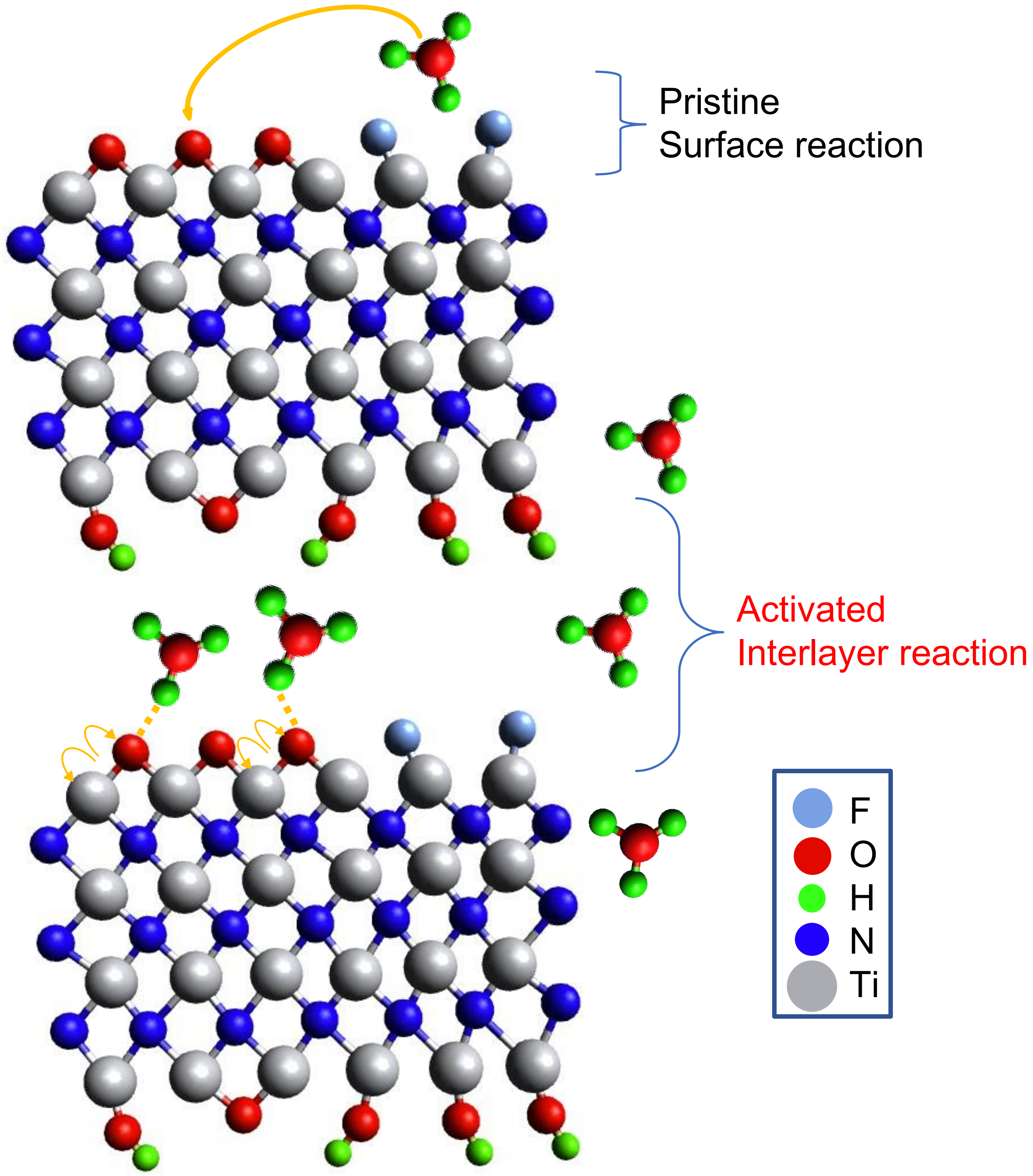
D. Johnson., A. Djire., et al. ChemElectroChem (2022)

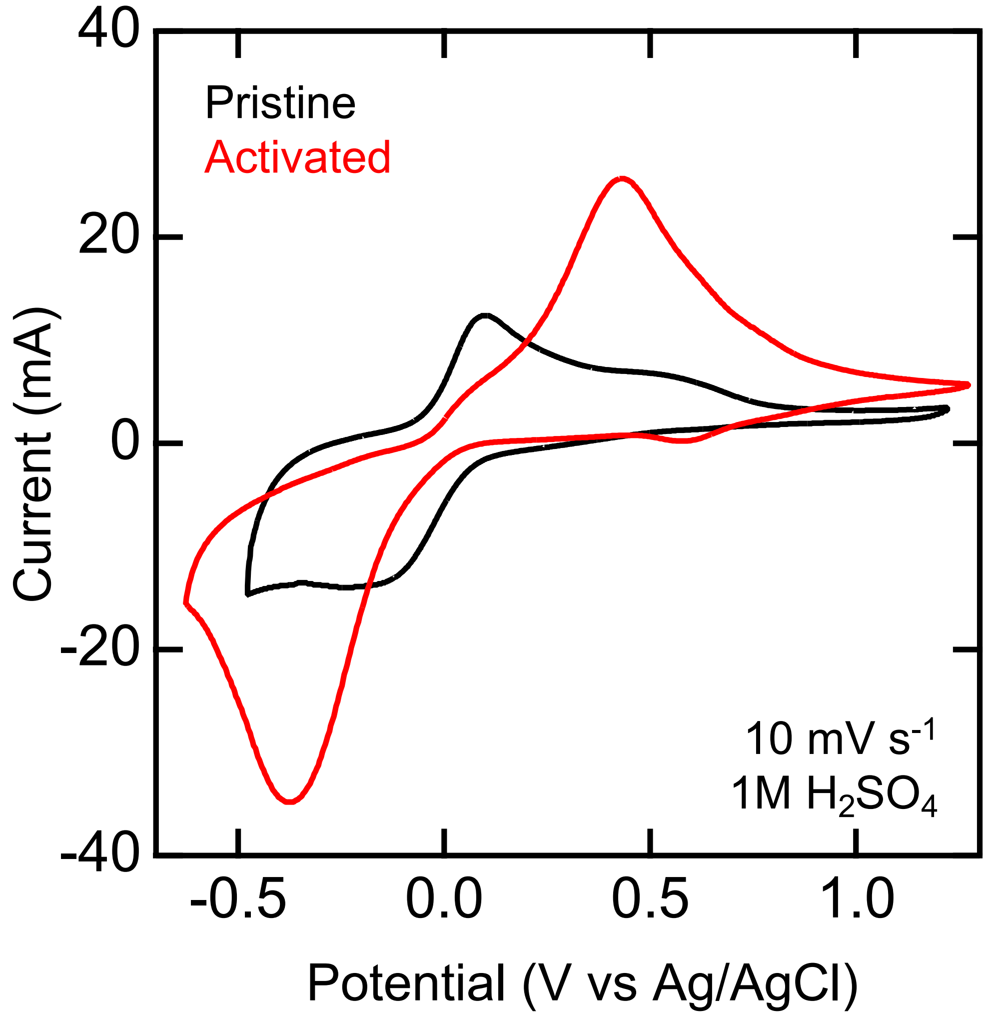


$$Ti - O - Ti + H^{+} + e^{-} \rightleftharpoons Ti - OH^{*} - Ti$$

Acidic Electrolyte (0.1M HCl)

MNenes for Energy Storage



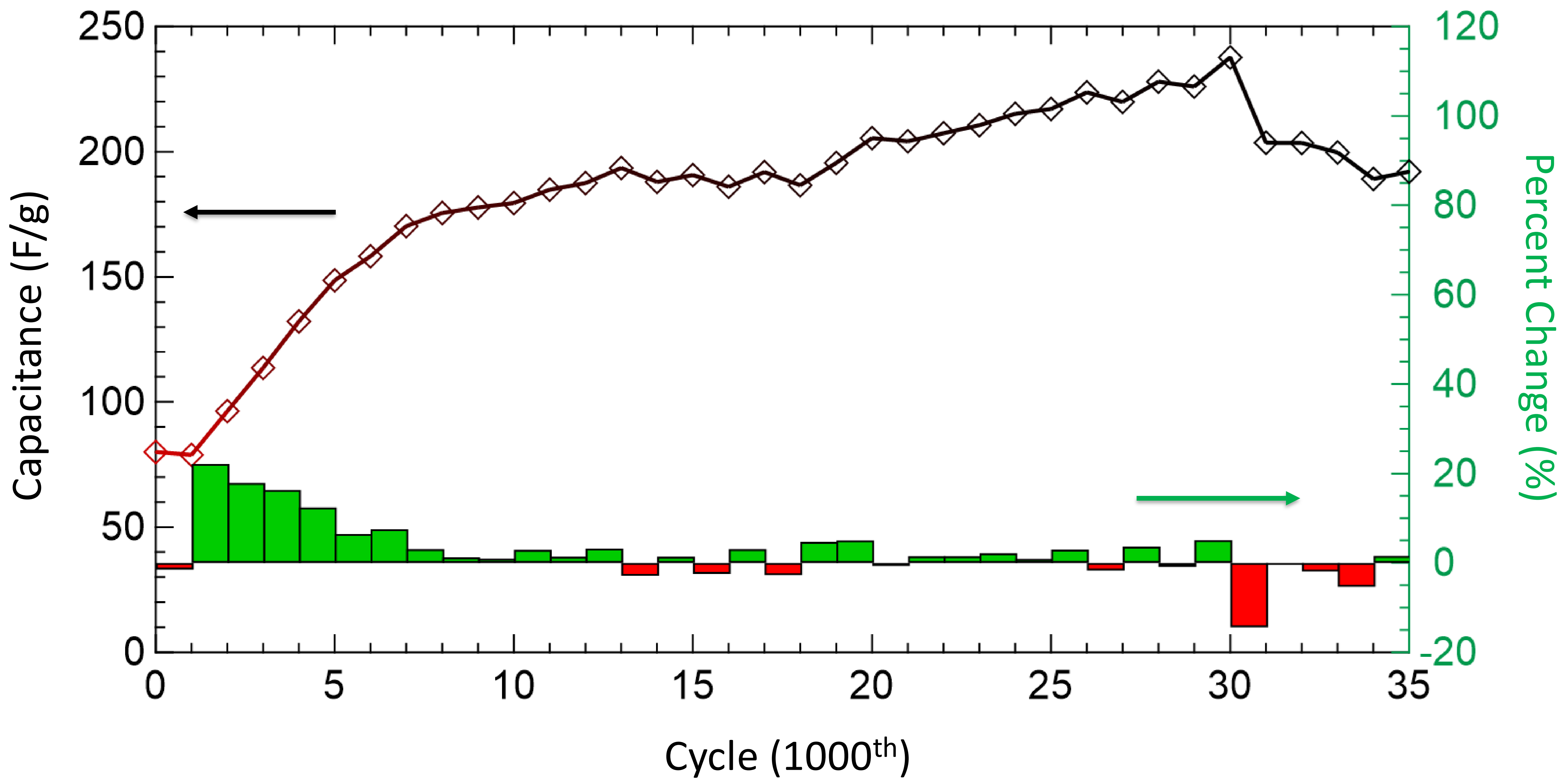


James Kasten

Ben Hsiao

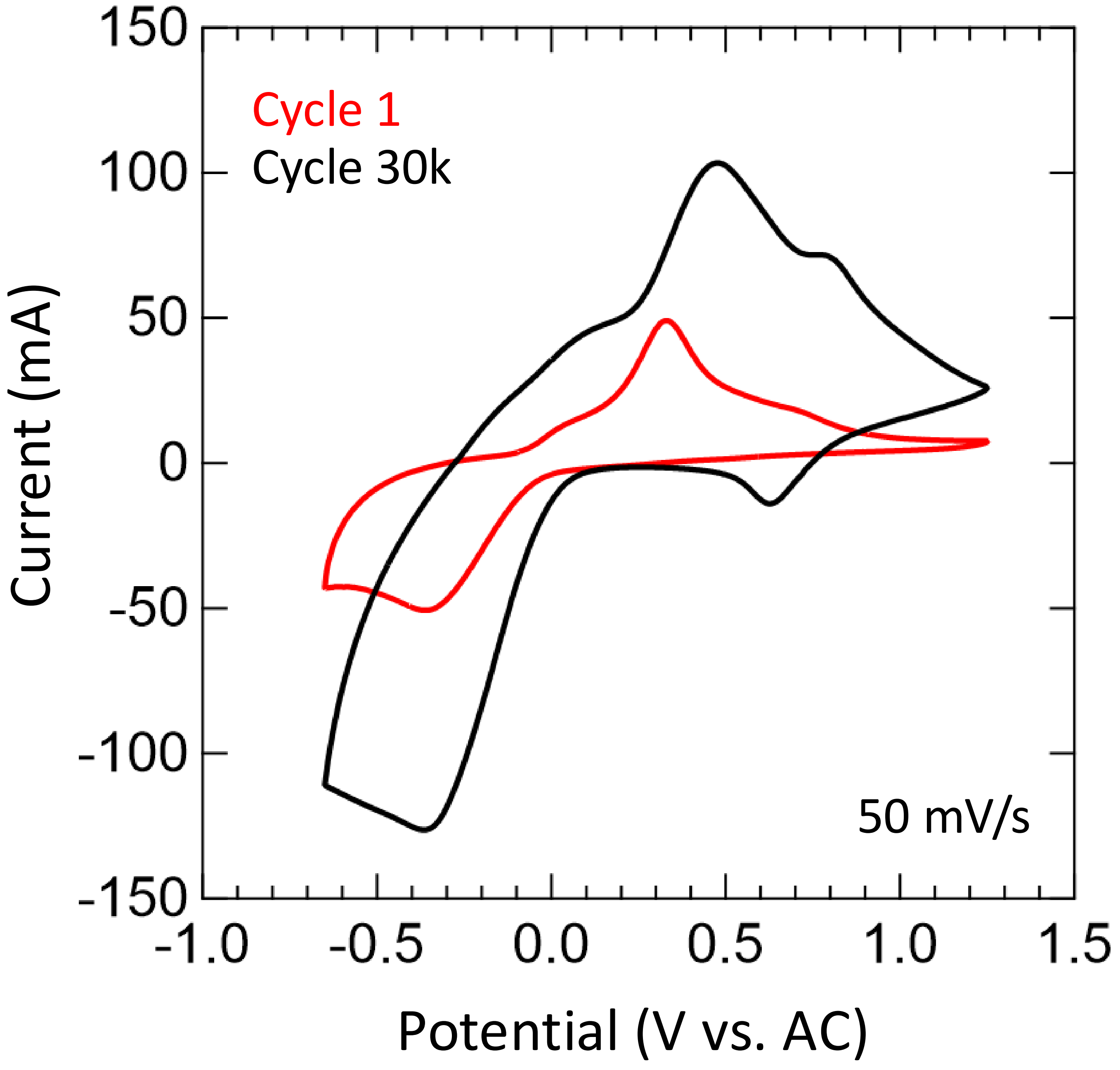
C. Hsiao, A. Djire, et. al., ACS Nano (2024)

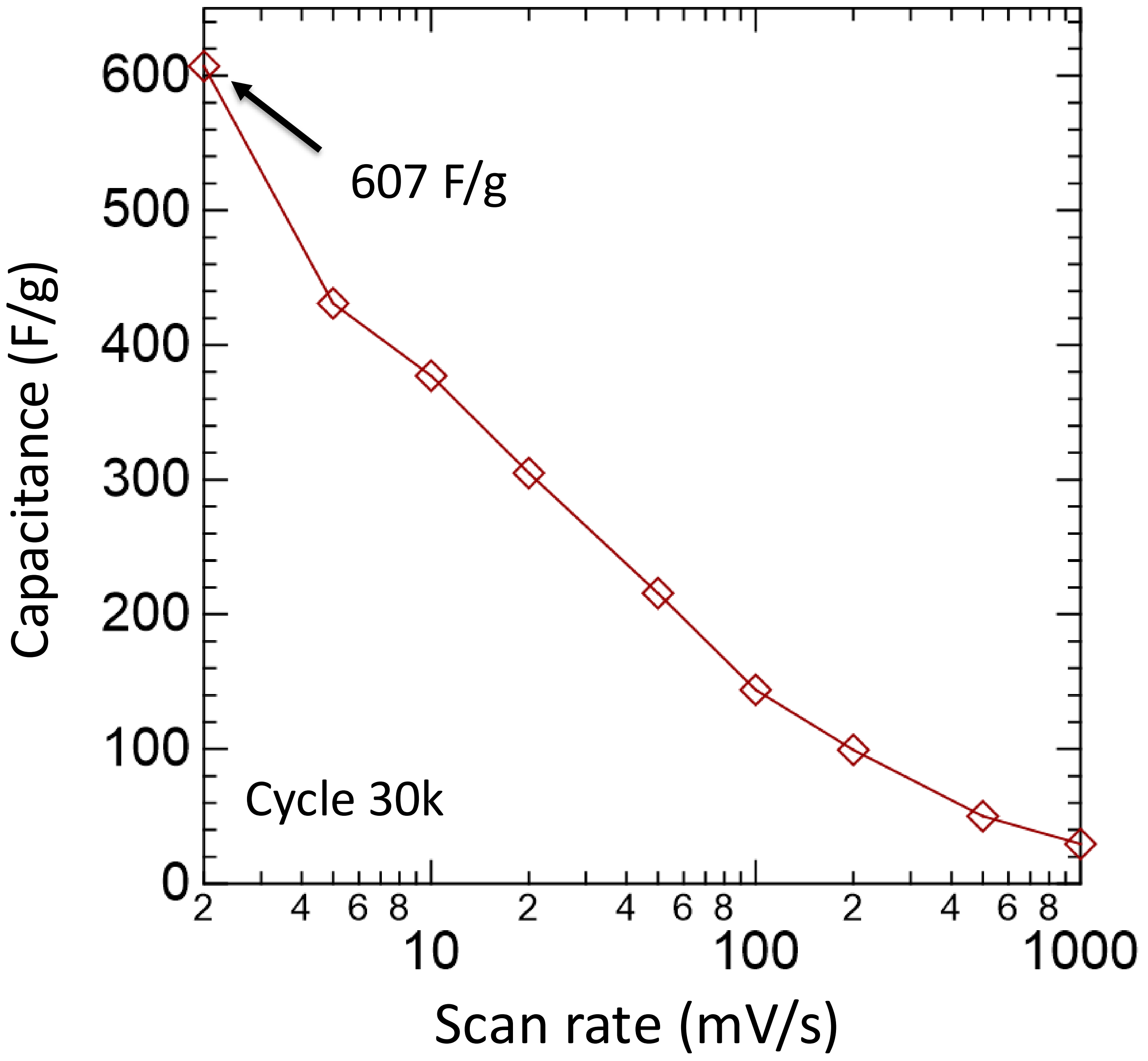
In-Situ Activation of MNenes



C. Hsiao, A. Djire, et. al., ACS Nano (2024)

High Capacitive Charge Storage





C. Hsiao, A. Djire, et. al., ACS Nano (2024)

U.S.-Africa Frontiers Symposium

Dalal Najib • 1st
Senior Director - Science and Engineering Capacity Development...
1yr •

The first US-Africa Frontiers of science, engineering and medicine symposium took place this week in Nairobi. A huge success with inspiring talks on cutting-edge research, outstanding part ...see more

Kingsley Obodo

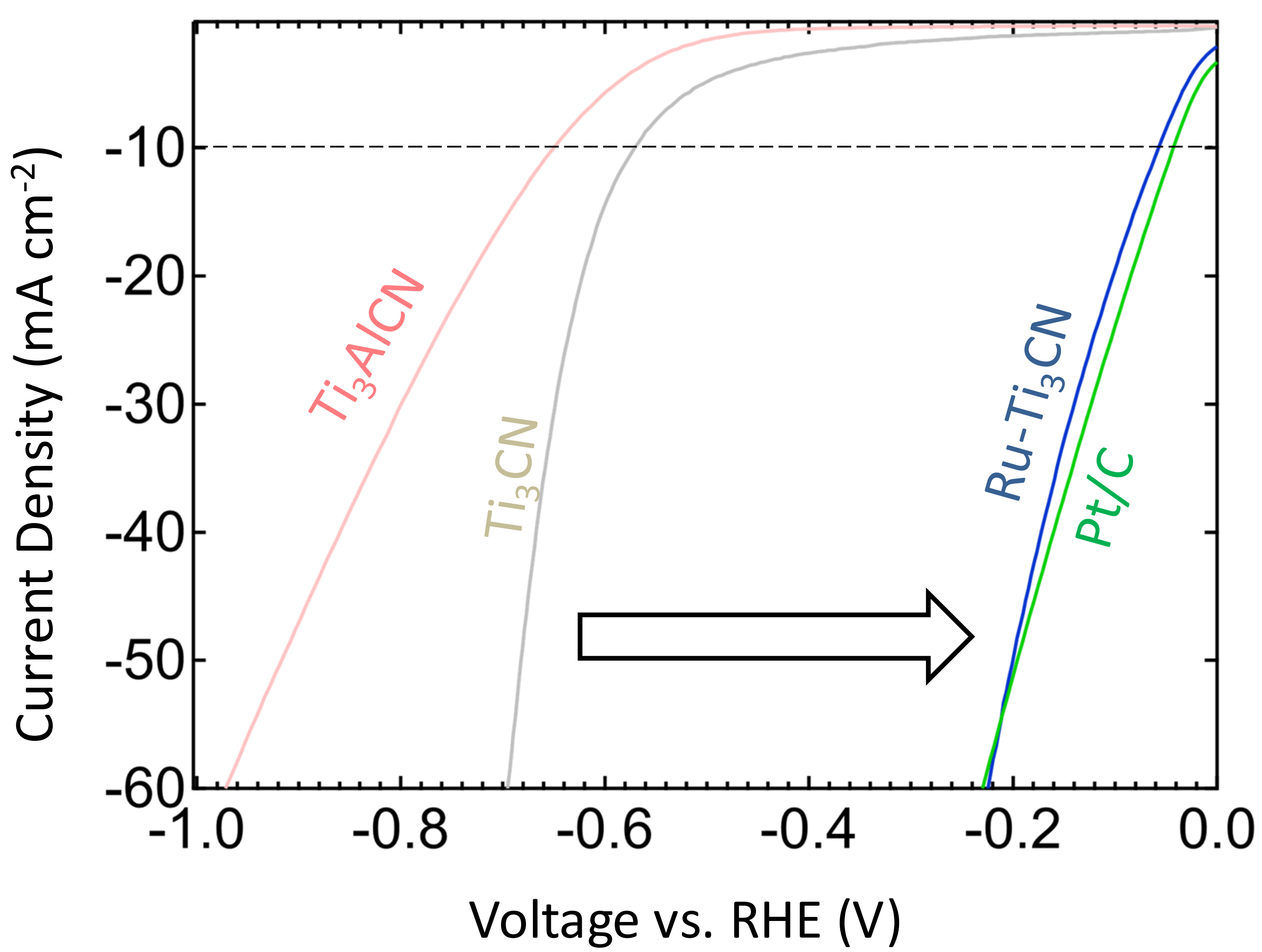
Hydrogen South Africa
North-West University

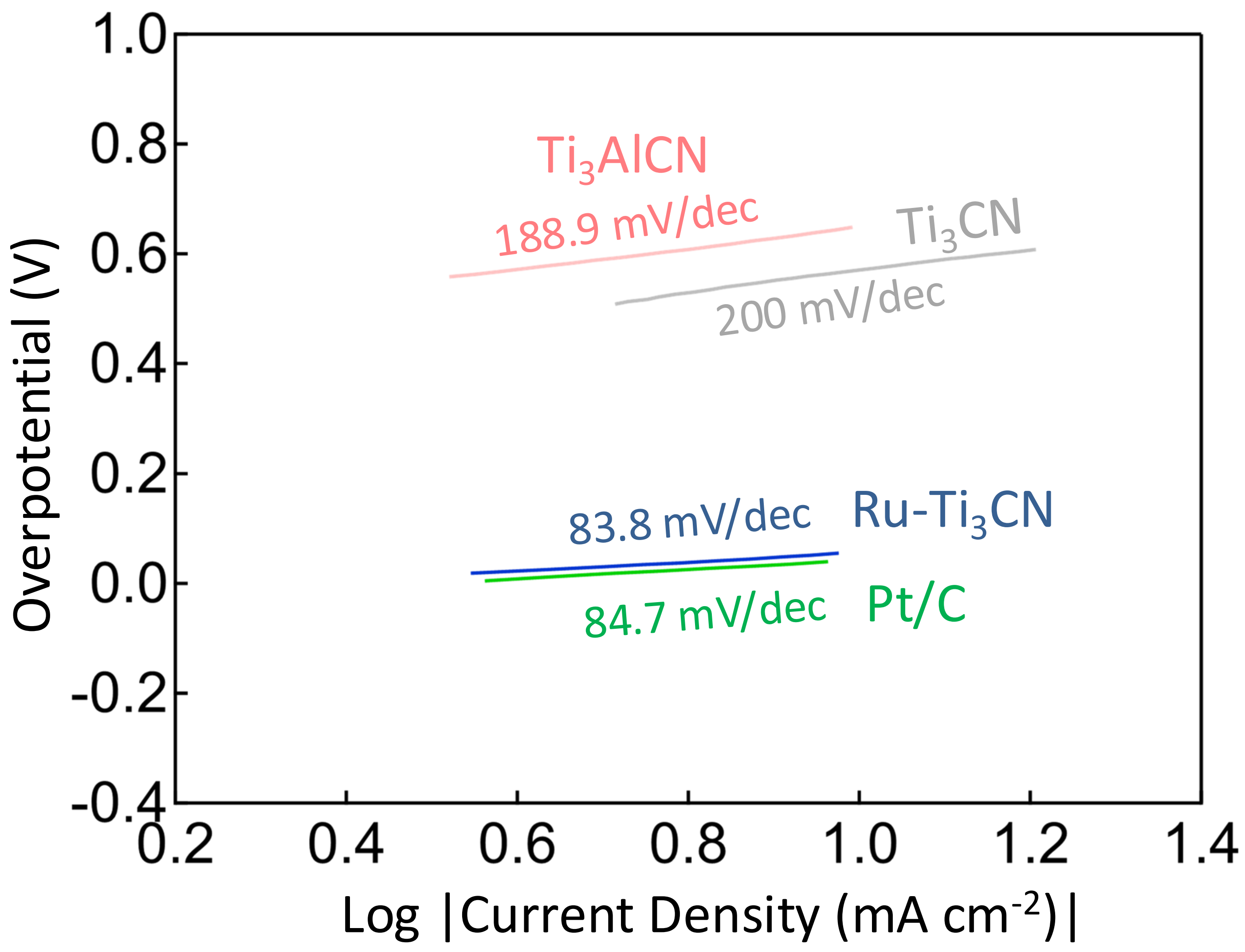
Balla Ngom

University Cheikh Anta
Diop of Dakar

HER activity of Ru-Ti_3CN MXene in Alkaline Electrolytes

Ru-Ti_3CN rivals Pt/C in performance and kinetics





Electrolyte: 0.5M KOH Reference electrode: Saturated Hg/HgO Counter electrode: Graphite rod

Uwadiunor, E, Obodo, K., Djire, A., et al. Chem Catalysis, 2023, 3, 100634

In Senegal


Abdoulaye Djire, PhD · You
Assistant Professor in Chemical Engineering at Texas A&M Uni...
4mo
Day 3 of my visit at the University Cheikh Anta Diop of Dakar. Enjoyed my meetings with Vice Dean Prof. Djop, and Department Heads of physics and chemistry Profs. Diao and Diouf. Big thanks to m ...see more


Abdoulaye Djire, PhD · You
Assistant Professor in Chemical Engineering at Texas A&M Uni...
4mo
Day 5 of my visit to the University Cheikh Anta Diop of Dakar, Seneg
Had a nice discussion with the Dean of the College of Sciences & Technologies, Prof. Bassirou Lo. Big thanks to my host and c ...see r


Abdoulaye Djire, PhD · You
Assistant Professor in Chemical Engineering at Texas A&M Uni...
3mo
Wrapping up week 2 of my visit to the University Cheikh Anta Diop of Dakar, Senegal. Enjoyed interacting with the students from the Ngom's group! Grateful to NASEM for the support!


Abdoulaye Djire, PhD · You
Assistant Professor in Chemical Engineering at Texas A&M Uni...
4mo
Day 1 of my visit at the University Cheikh Anta Diop of Dakar, Senegal. Super excited to be working with the group of Dr. Balla Ngom and his amazing students. We are establishing the first 2D MXene re ...see more

In Burkina Faso

In Mali

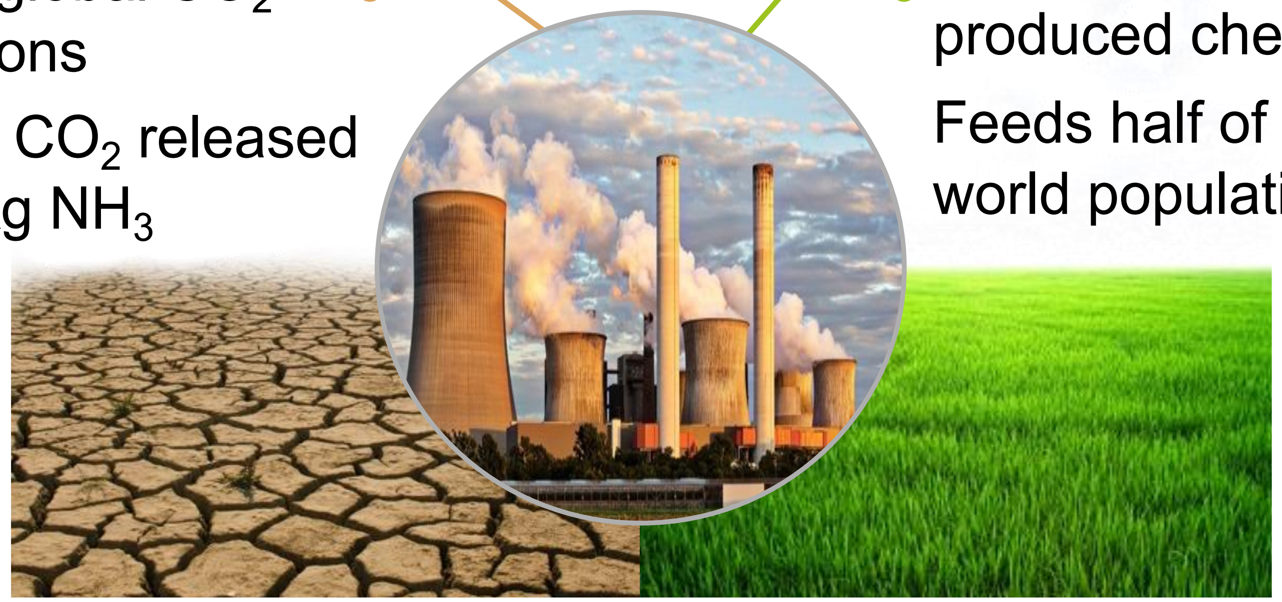
Faculty of Sciences

World Ammonia Production *via* Thermochemistry

Negative

1% of global CO_2 emissions

1.6 Kg CO_2 released per 1Kg NH_3

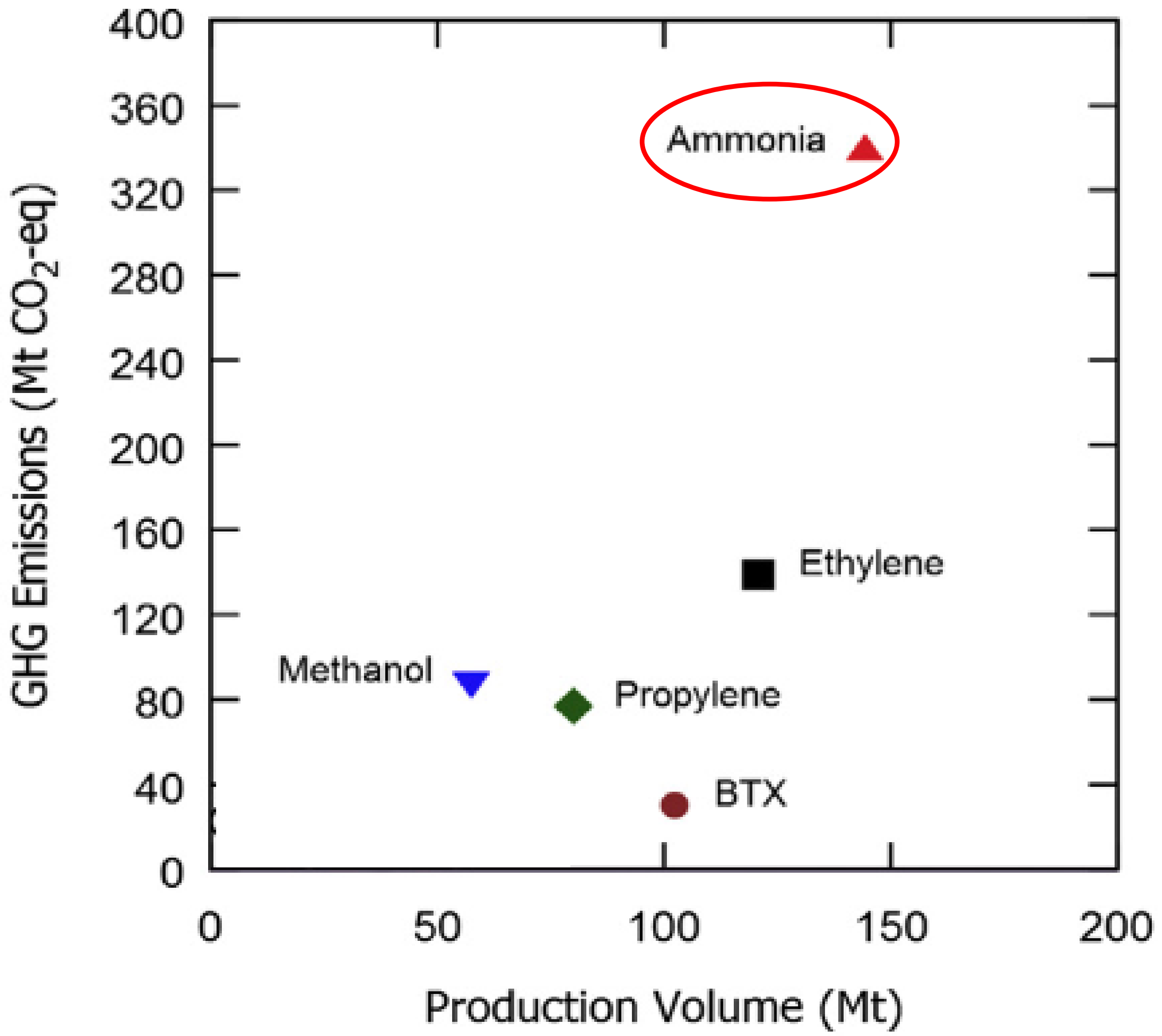


Positive

NH_3: 2nd most produced chemical

Feeds half of the world population

Industrial ammonia production emits more CO_2 than any other chemical-making reaction

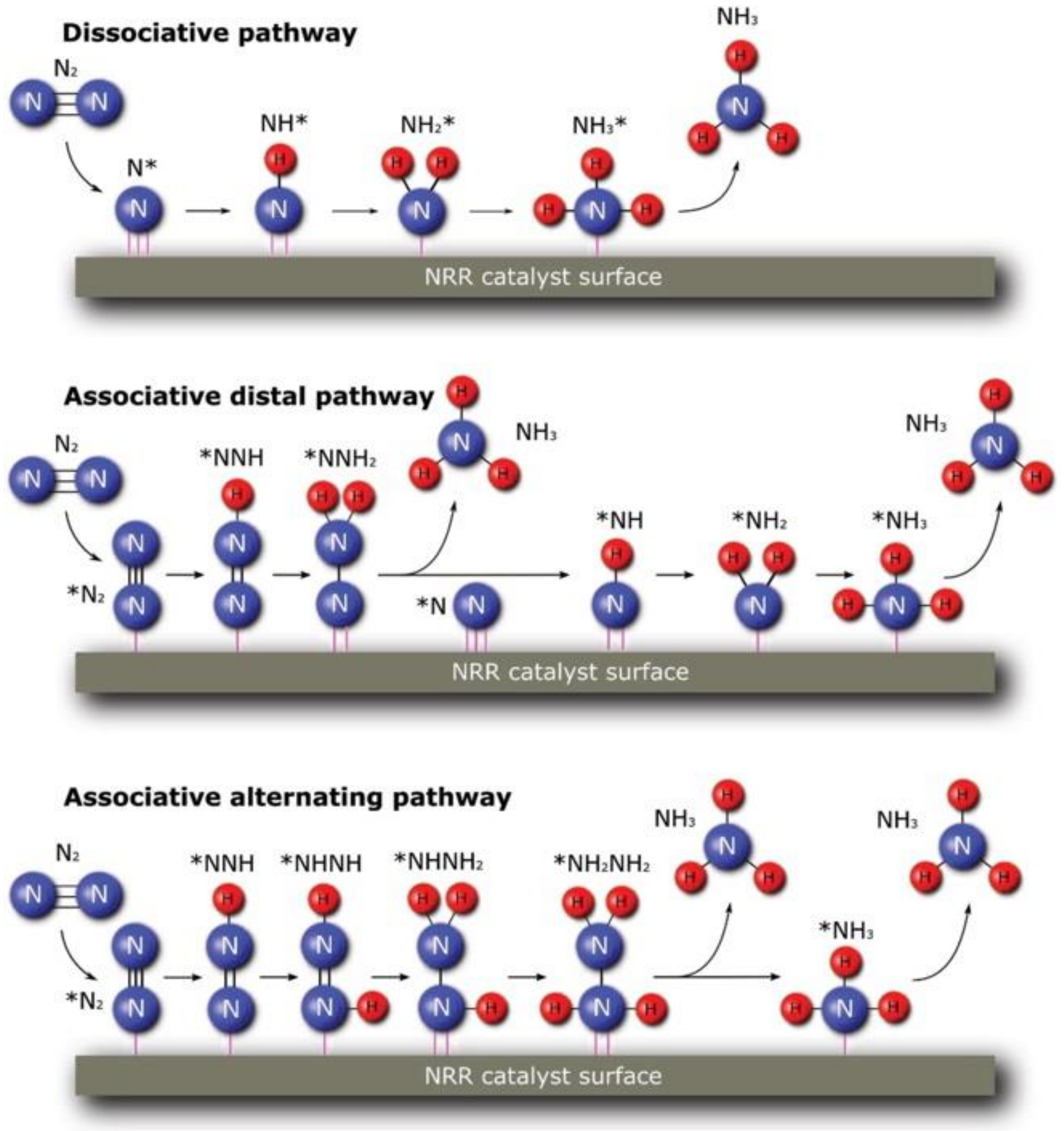


Current Target for Practical Application ≥ **60% Selectivity (or Faradaic Efficiency)**

Djire, A., et al. Cell Reports Phys. Sci. 2021, 2, 5, 100438

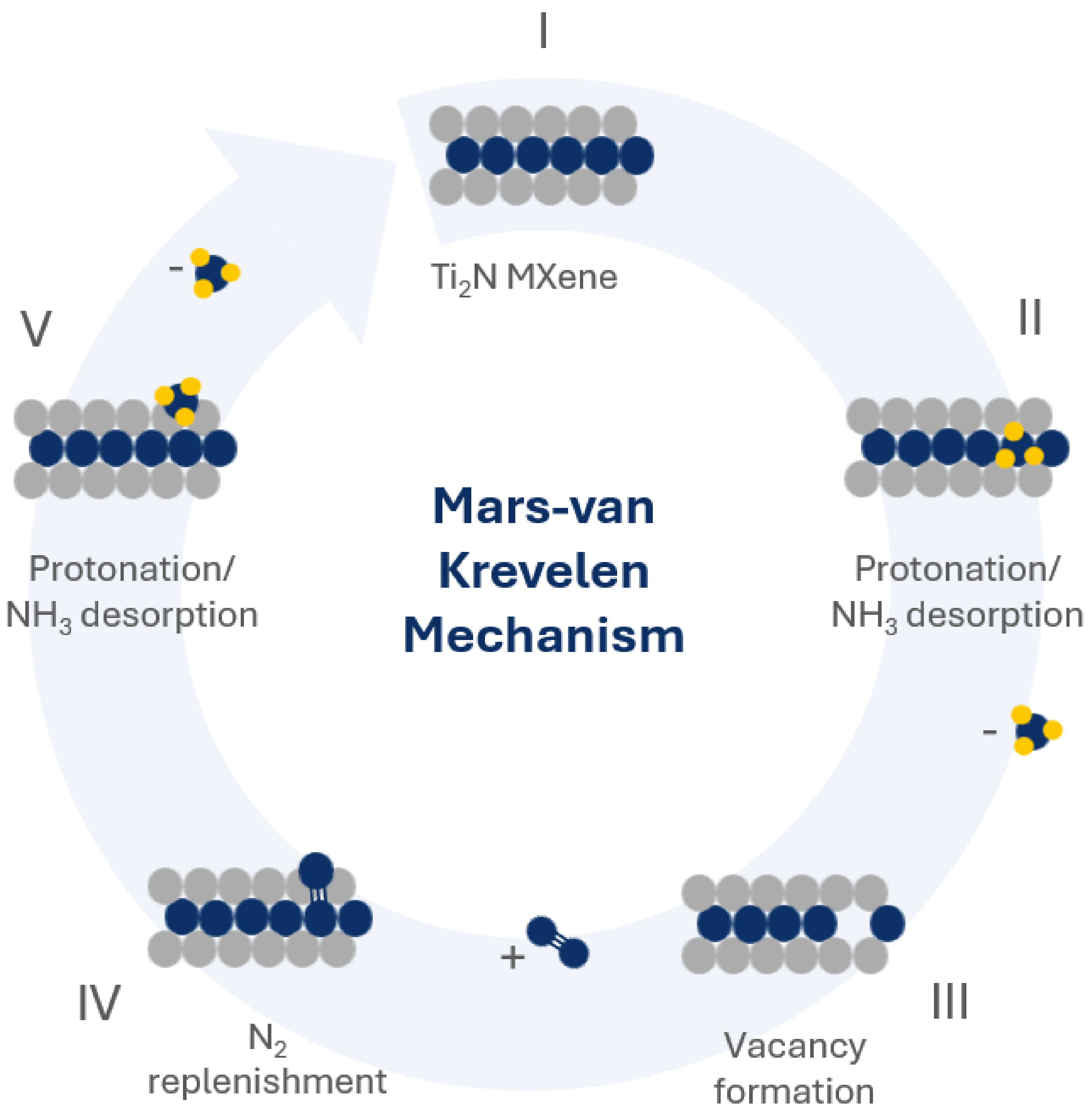
Manthiram, K., et al., Joule 2017, 1, 10-14

Conventional Approach Suffers From Low Efficiency



- Explored catalysts are:
  - Single-atom catalysts
  - Pure metal hybrid clusters
  - Perovskites
  - Transition metal carbides, oxides, nitrides, sulfides
- Suffer from HER surface competition resulting in low FE
- Sluggish and kinetically limited

Our Approach of Ammonia Synthesis via MvK Mechanism



- ❑ Lattice N atoms are involved in the electrochemical formation of NH_3
- ❑ Is the formation and replenishment of N vacancies a stable cycle?

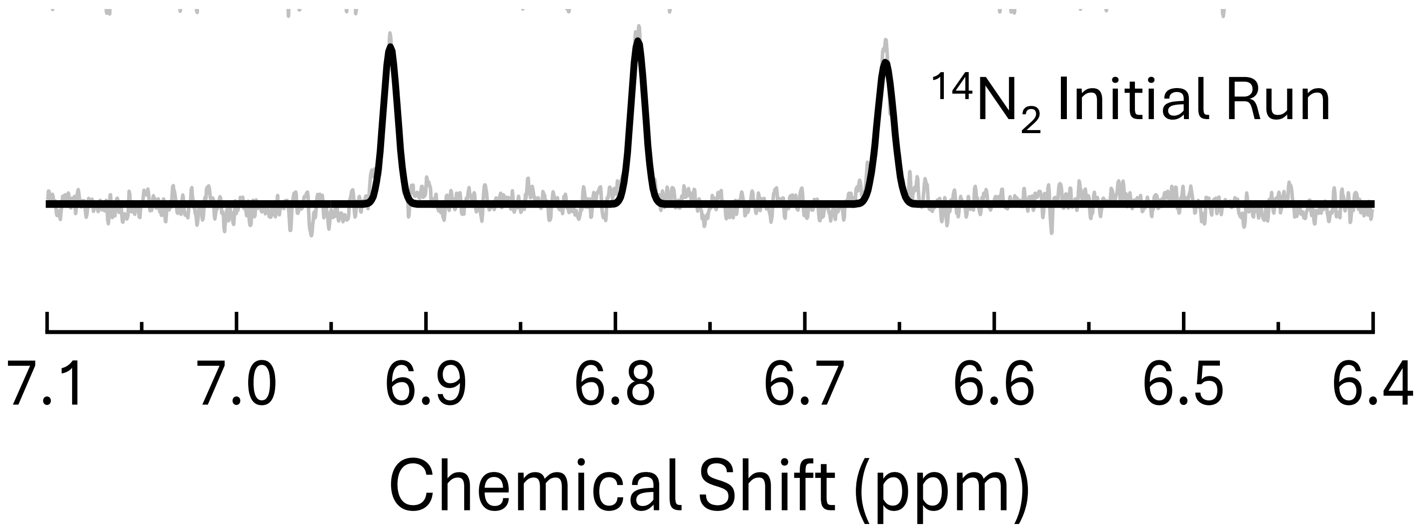
Denis Johnson

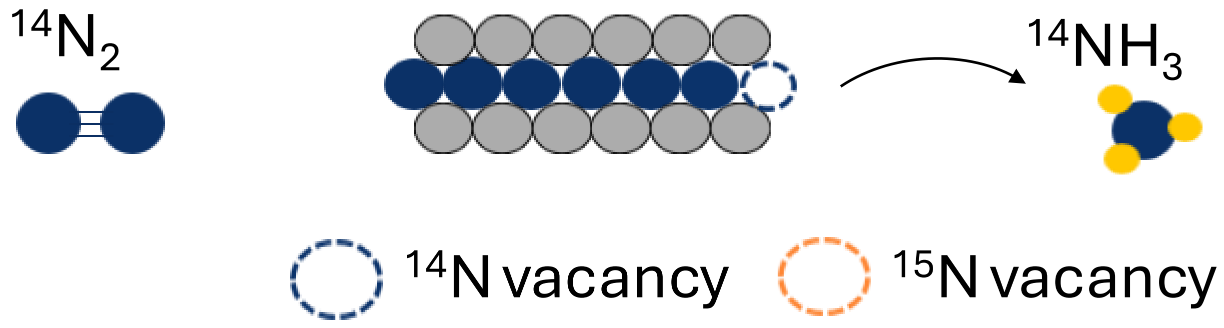
David Kumar

Djire et al., J. Am. Chem. Soc. 2025, 147, 29327–29339

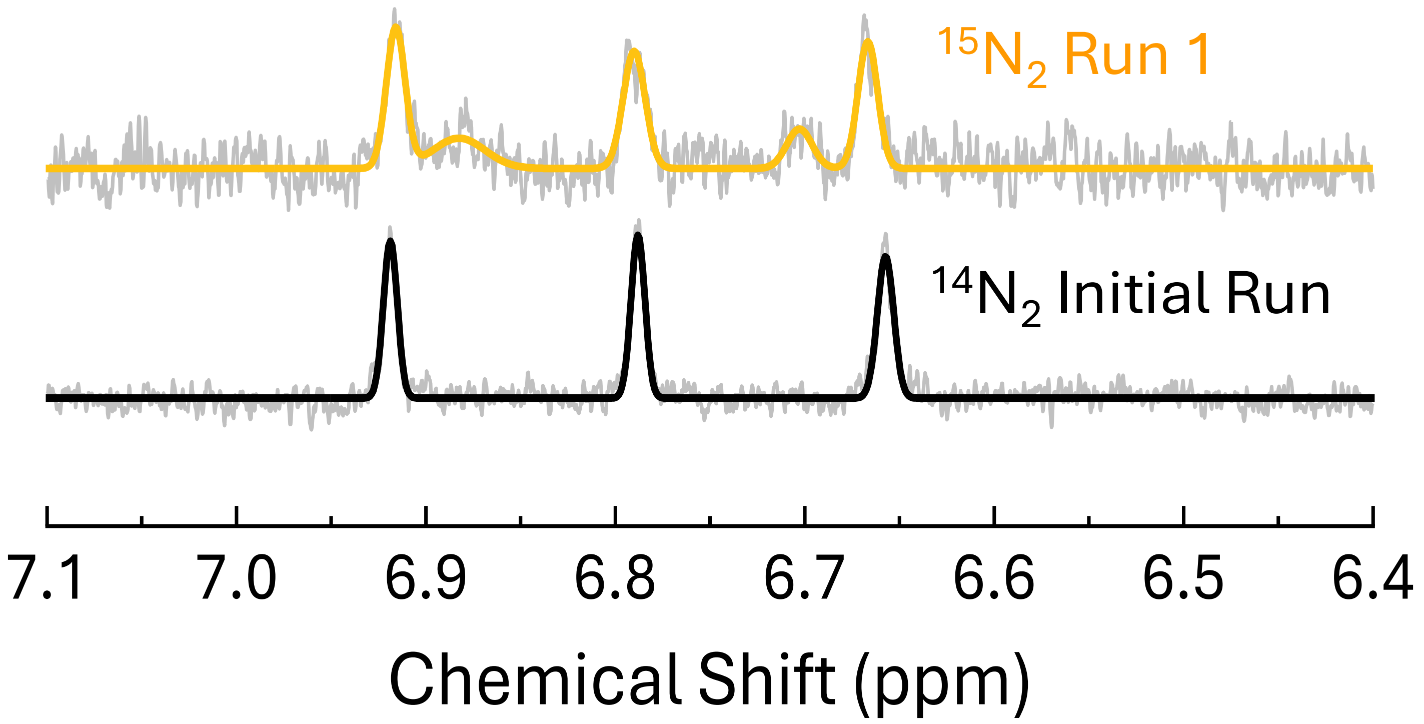
Probing MvK Mechanism via NMR Analysis

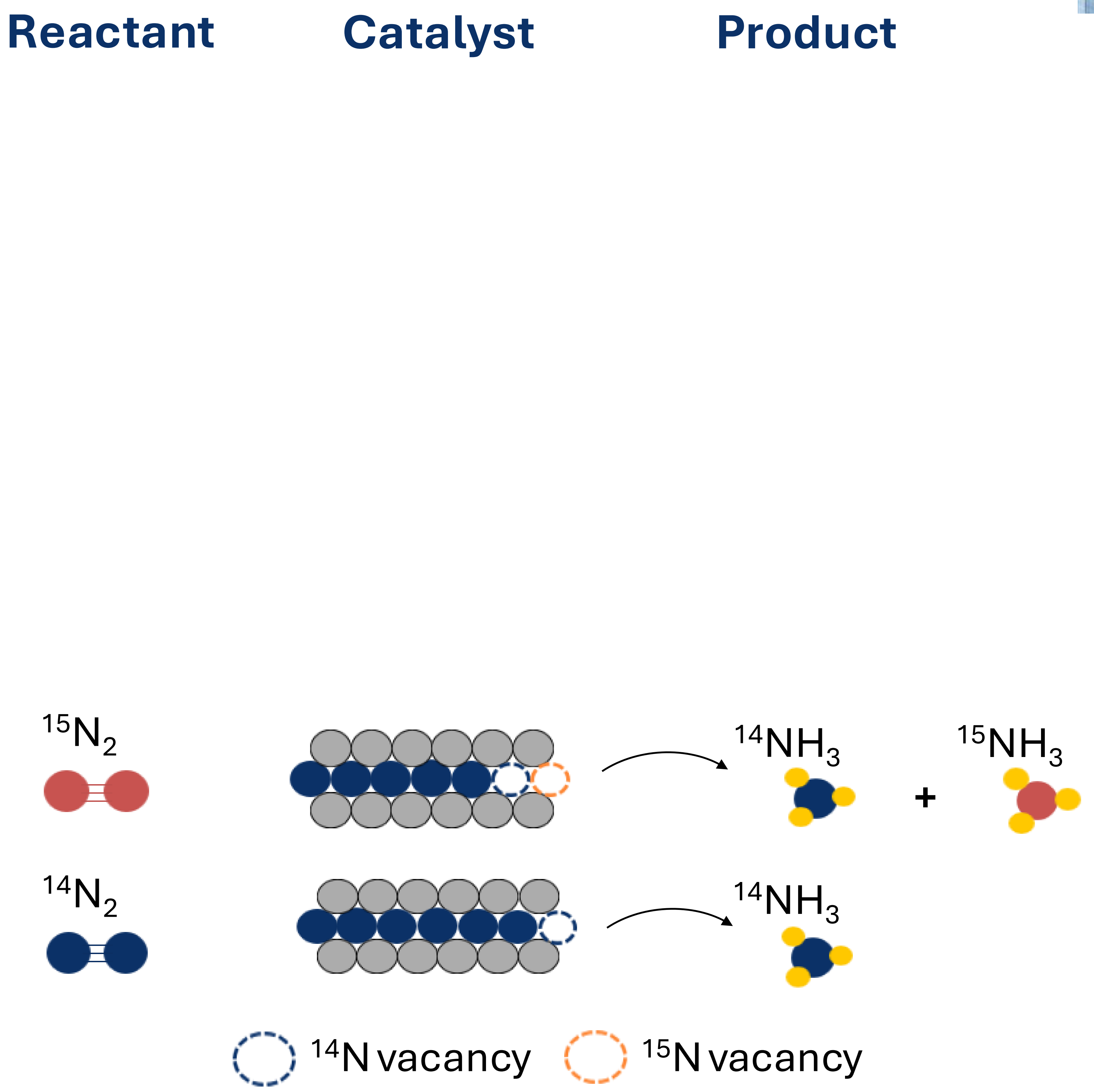
Reactant **Catalyst** **Product**





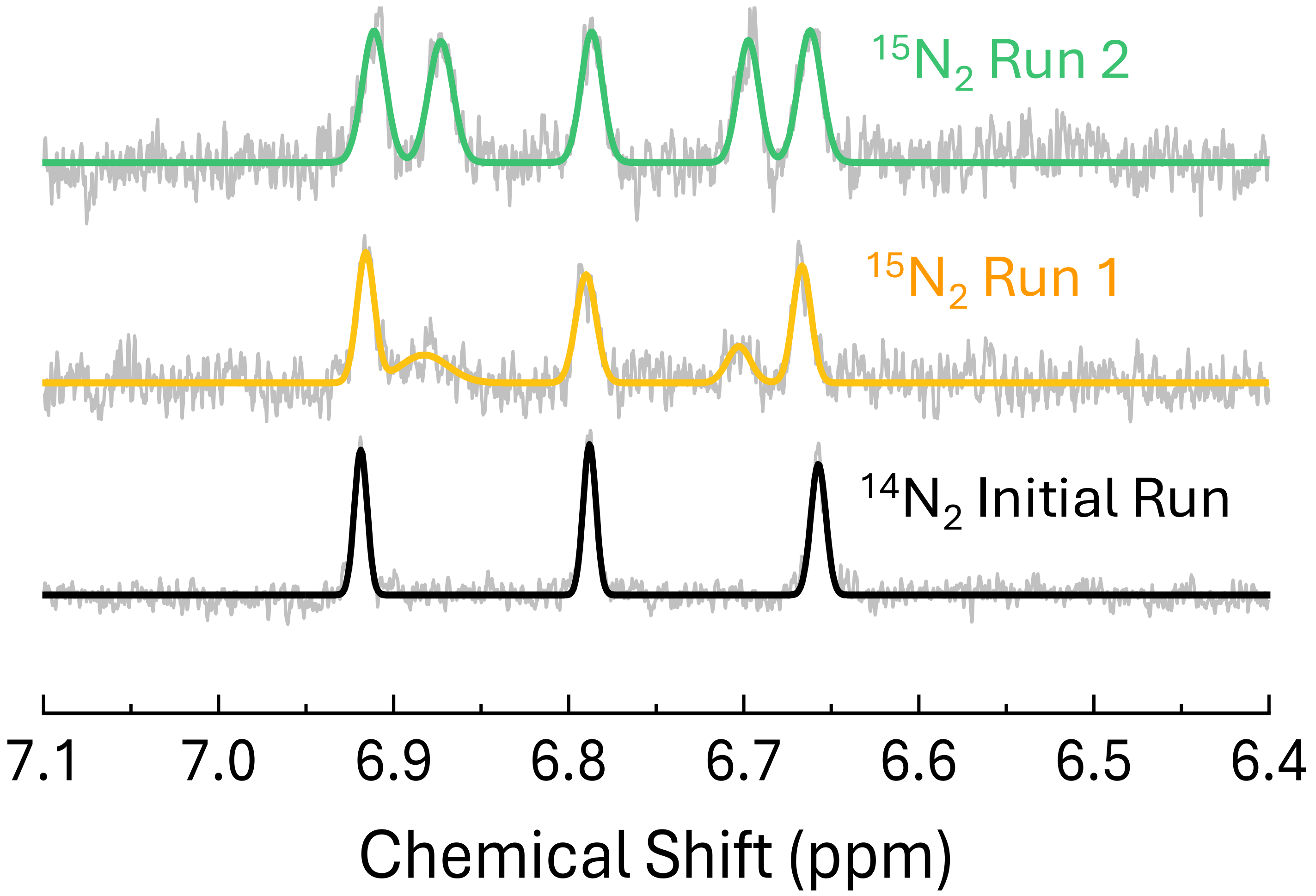
Probing MvK Mechanism via NMR Analysis

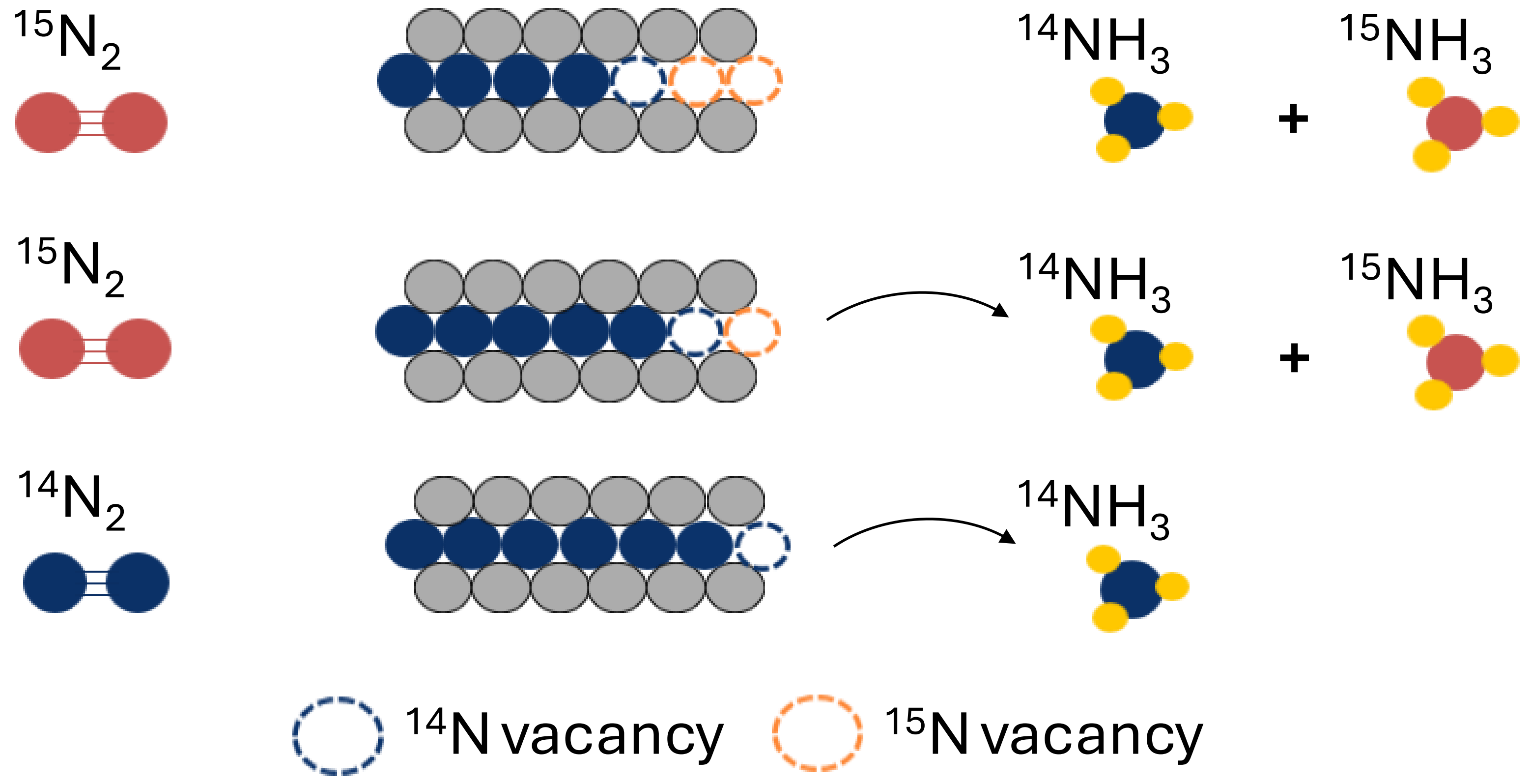




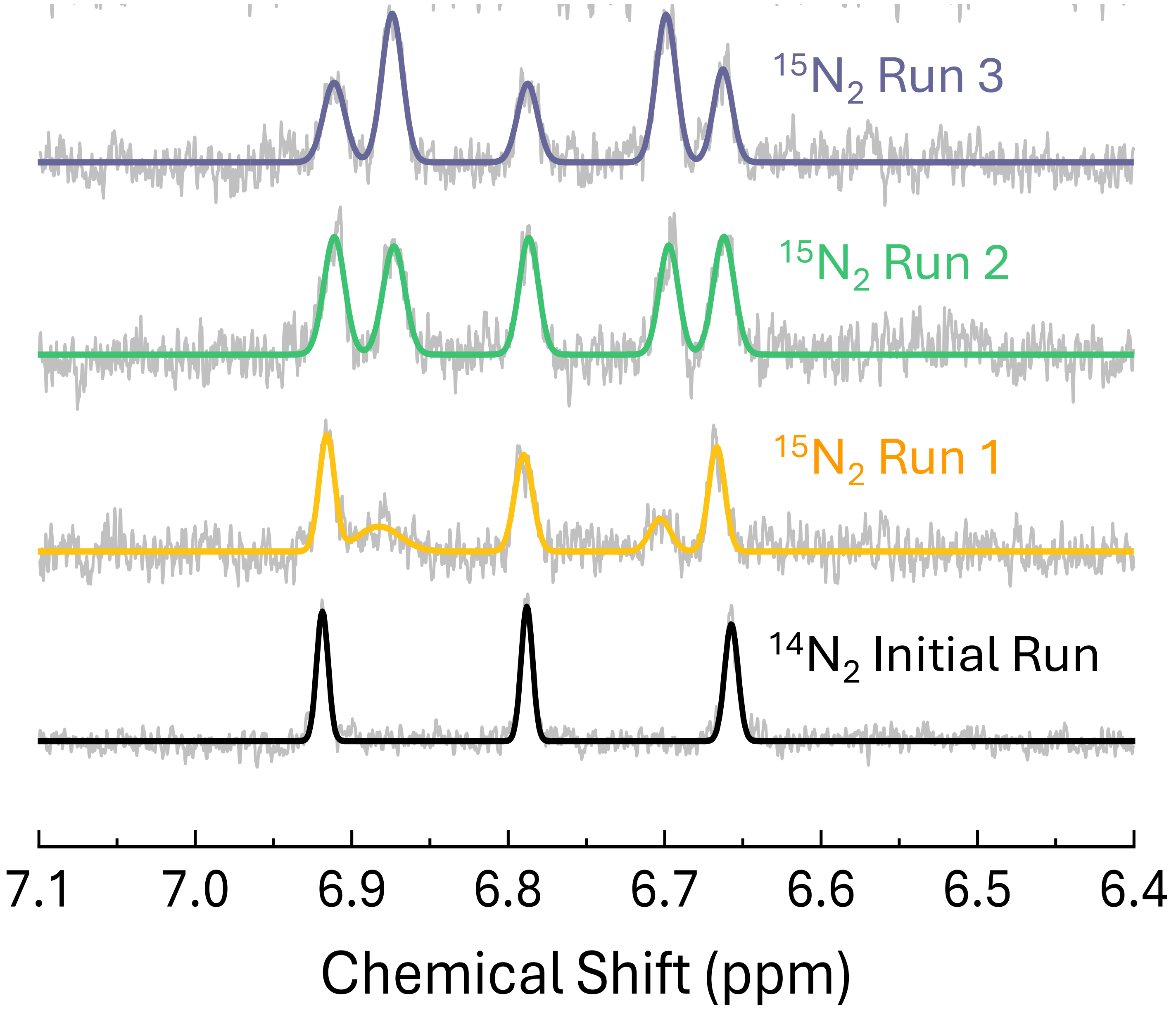
Probing MvK Mechanism via NMR Analysis

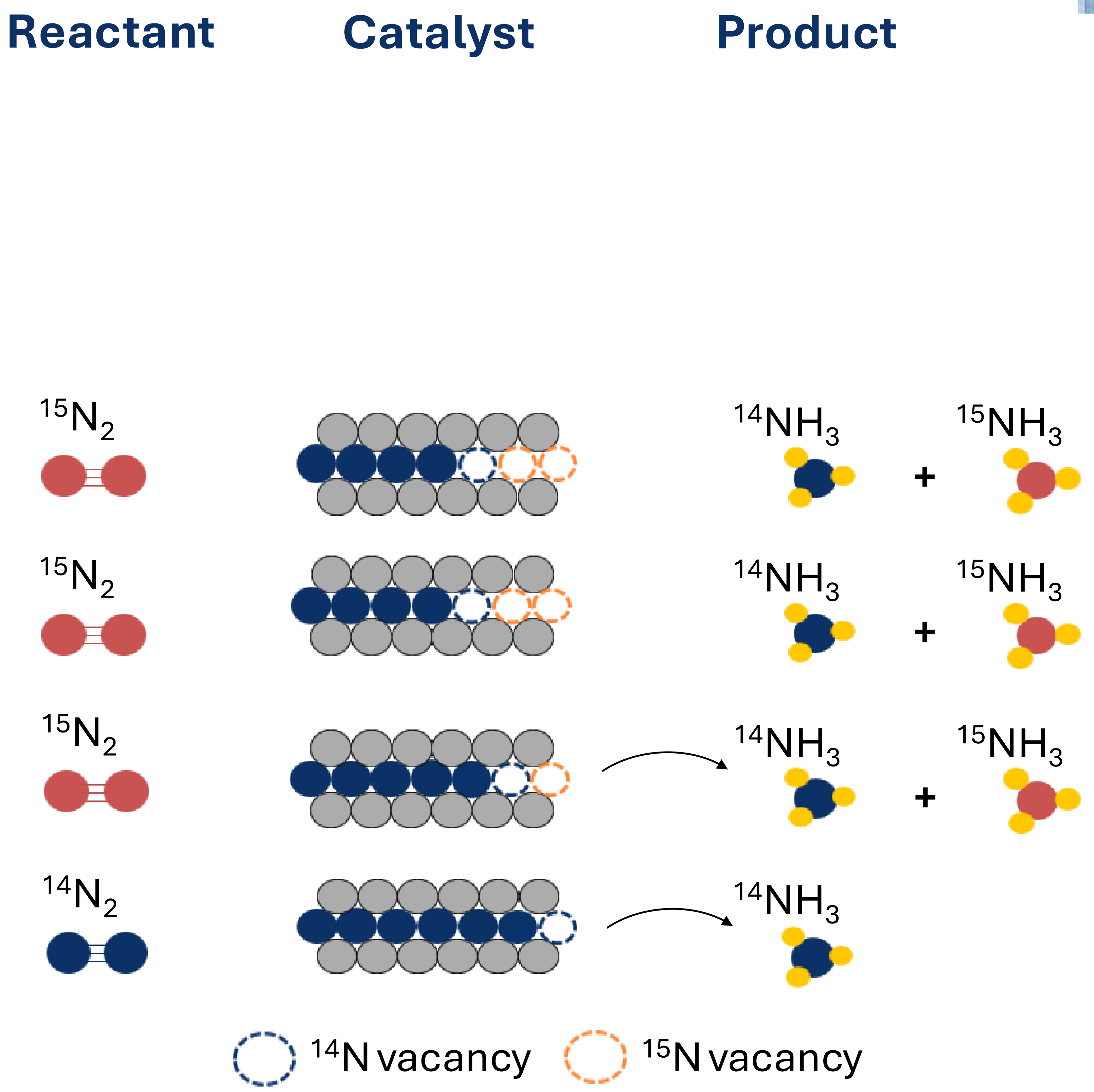
Reactant **Catalyst** **Product**



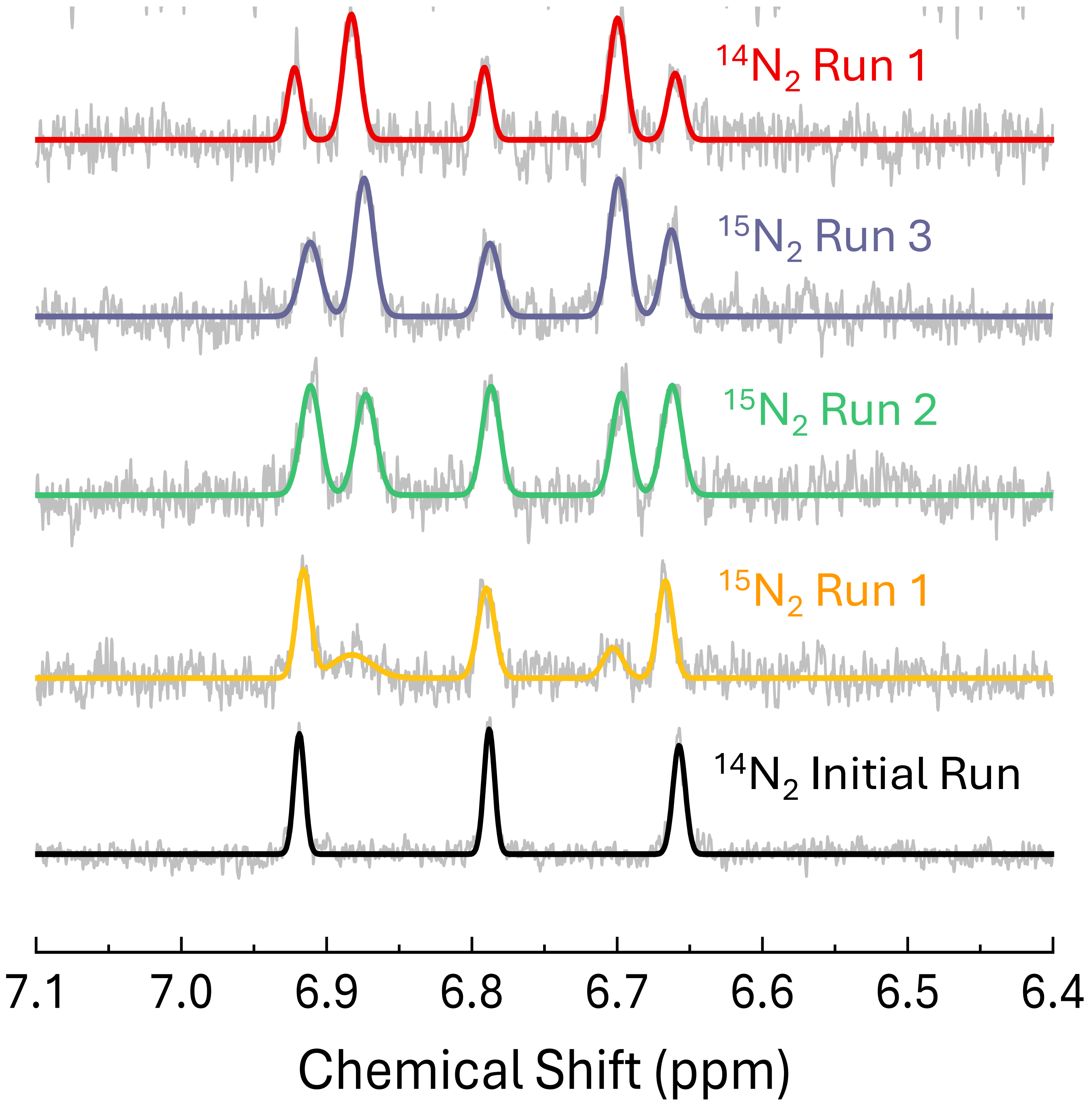


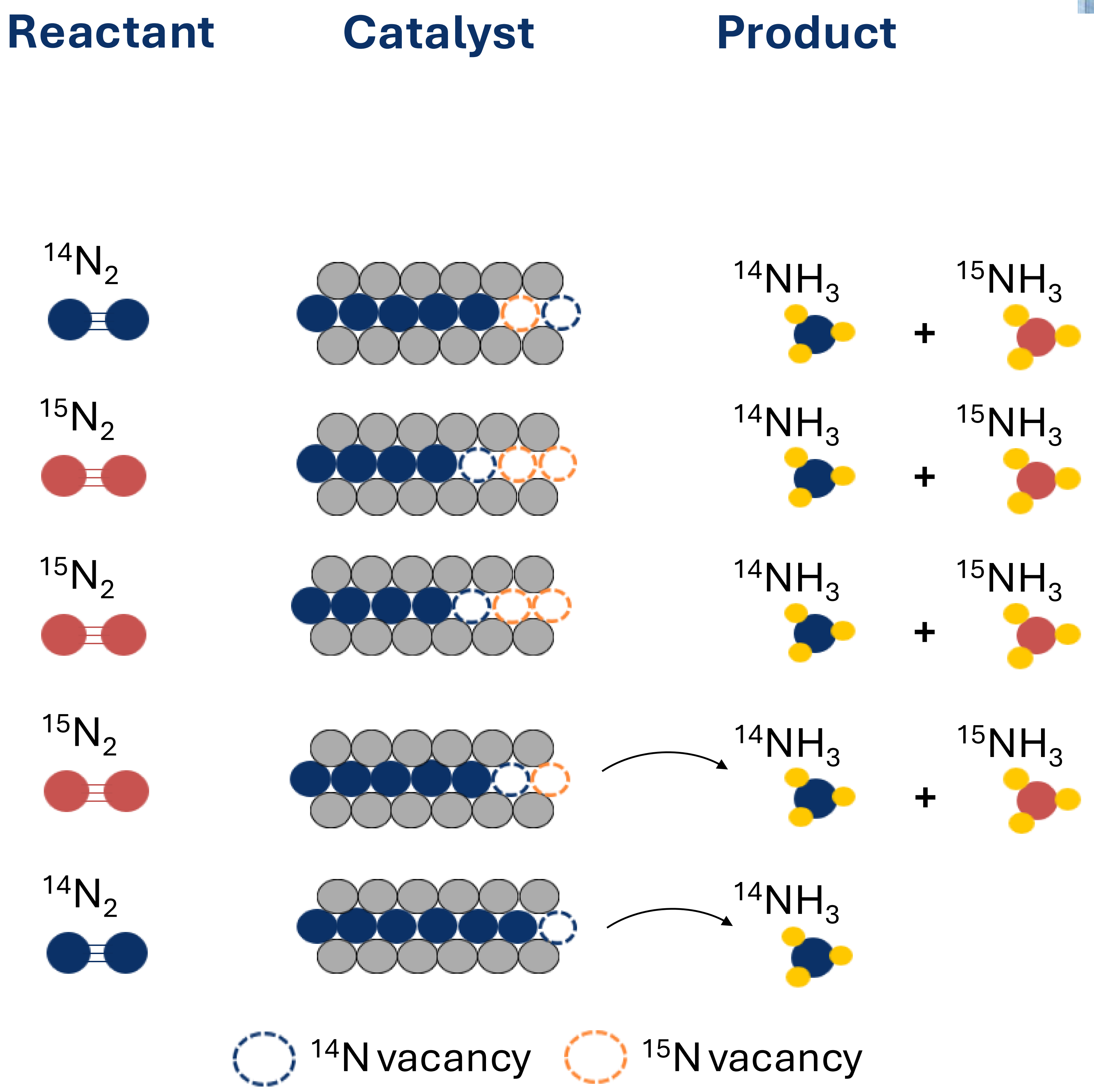
Probing MvK Mechanism via NMR Analysis



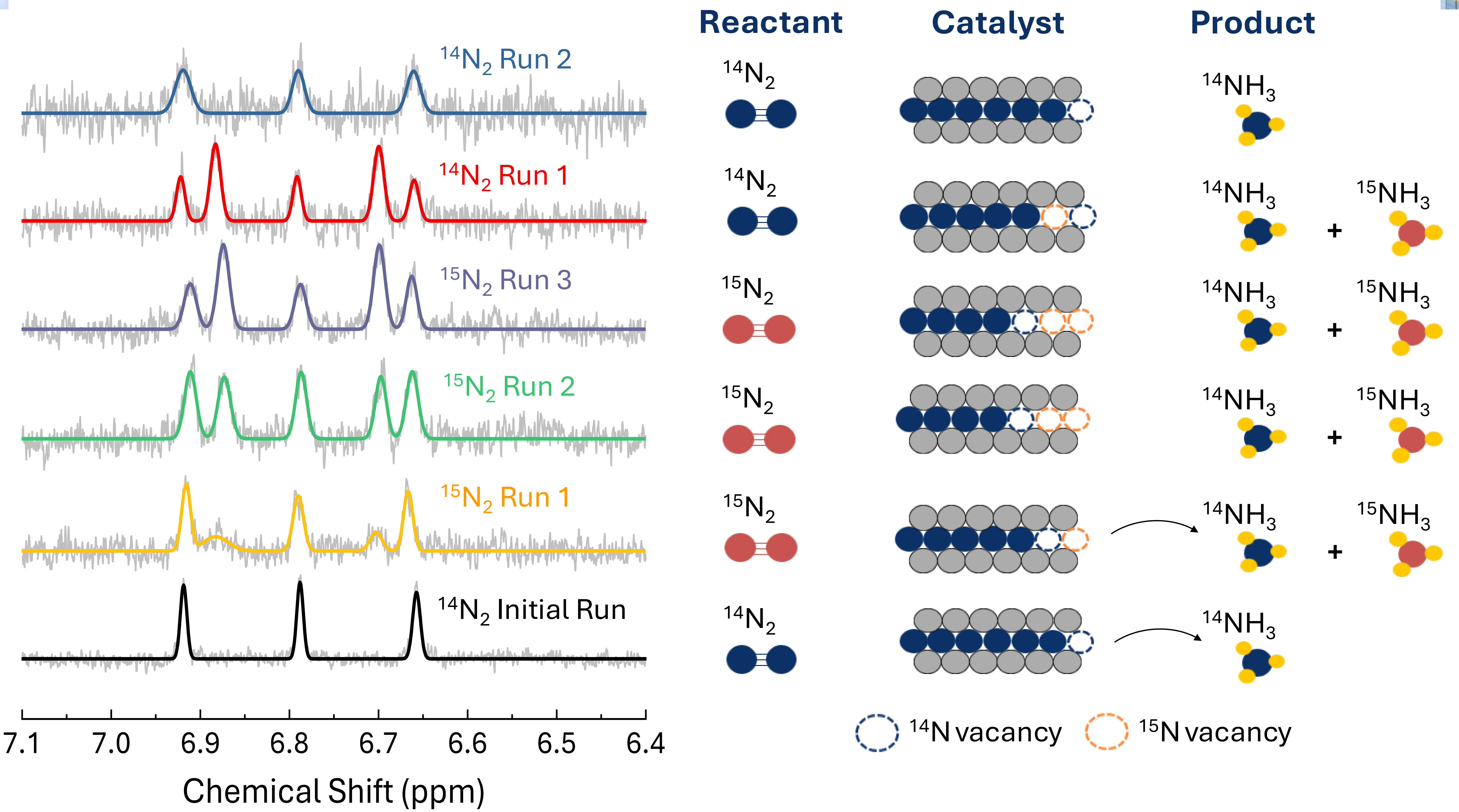


Probing MvK Mechanism via NMR Analysis

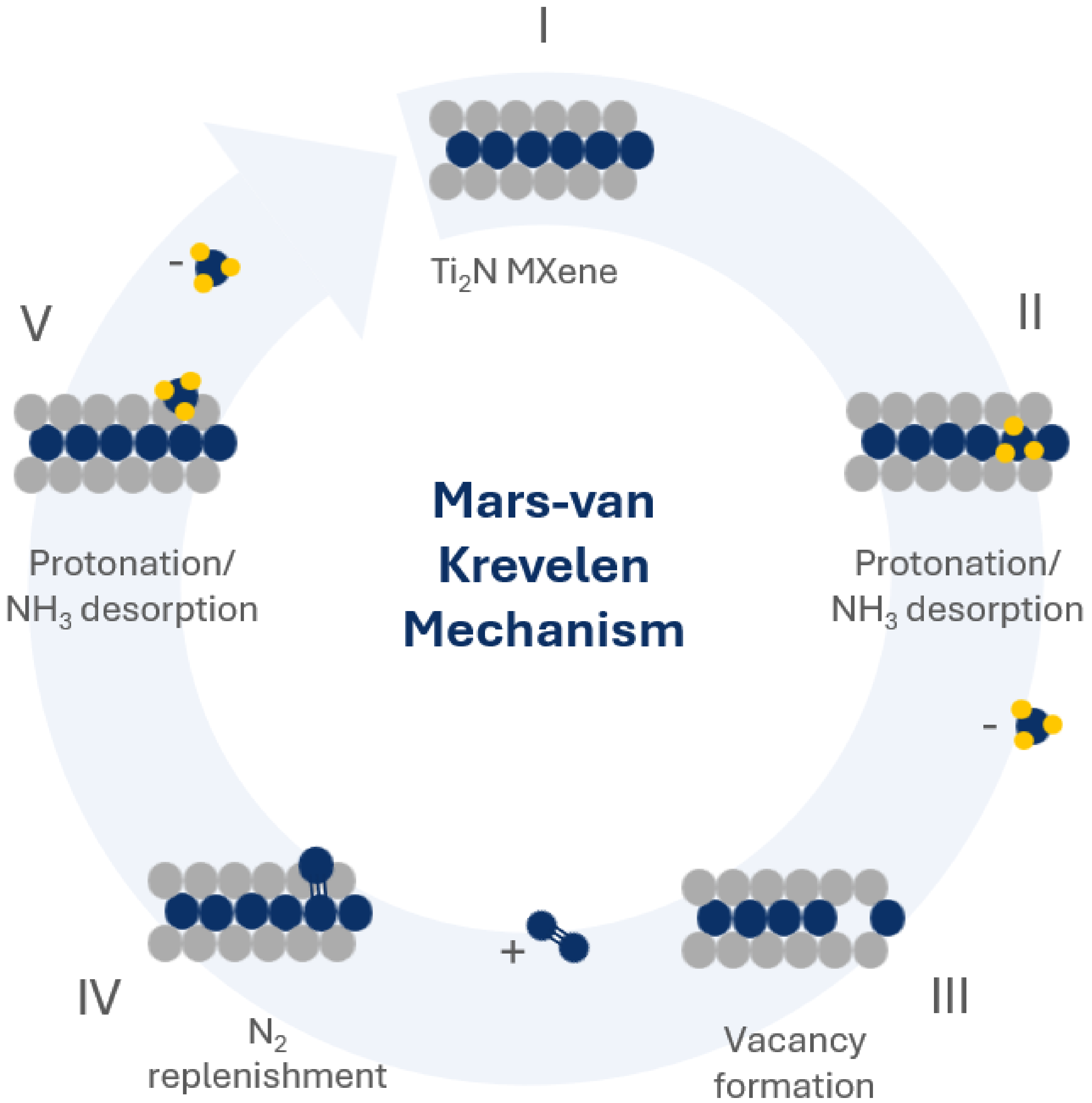




Probing MvK Mechanism via NMR Analysis



Our Approach of Ammonia Synthesis via MvK Mechanism

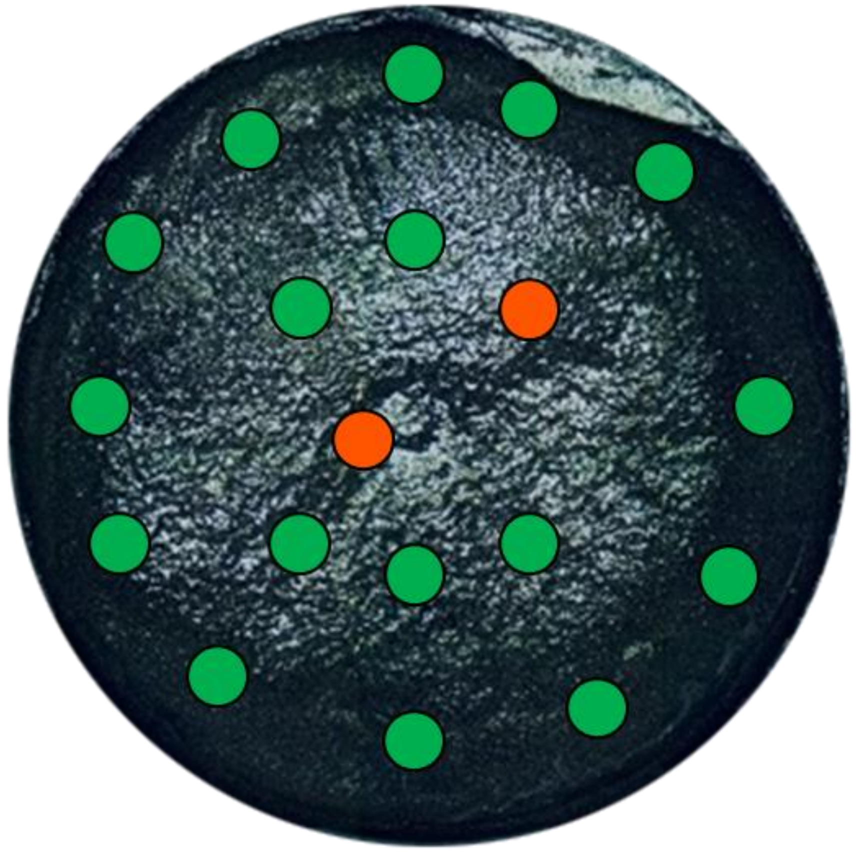


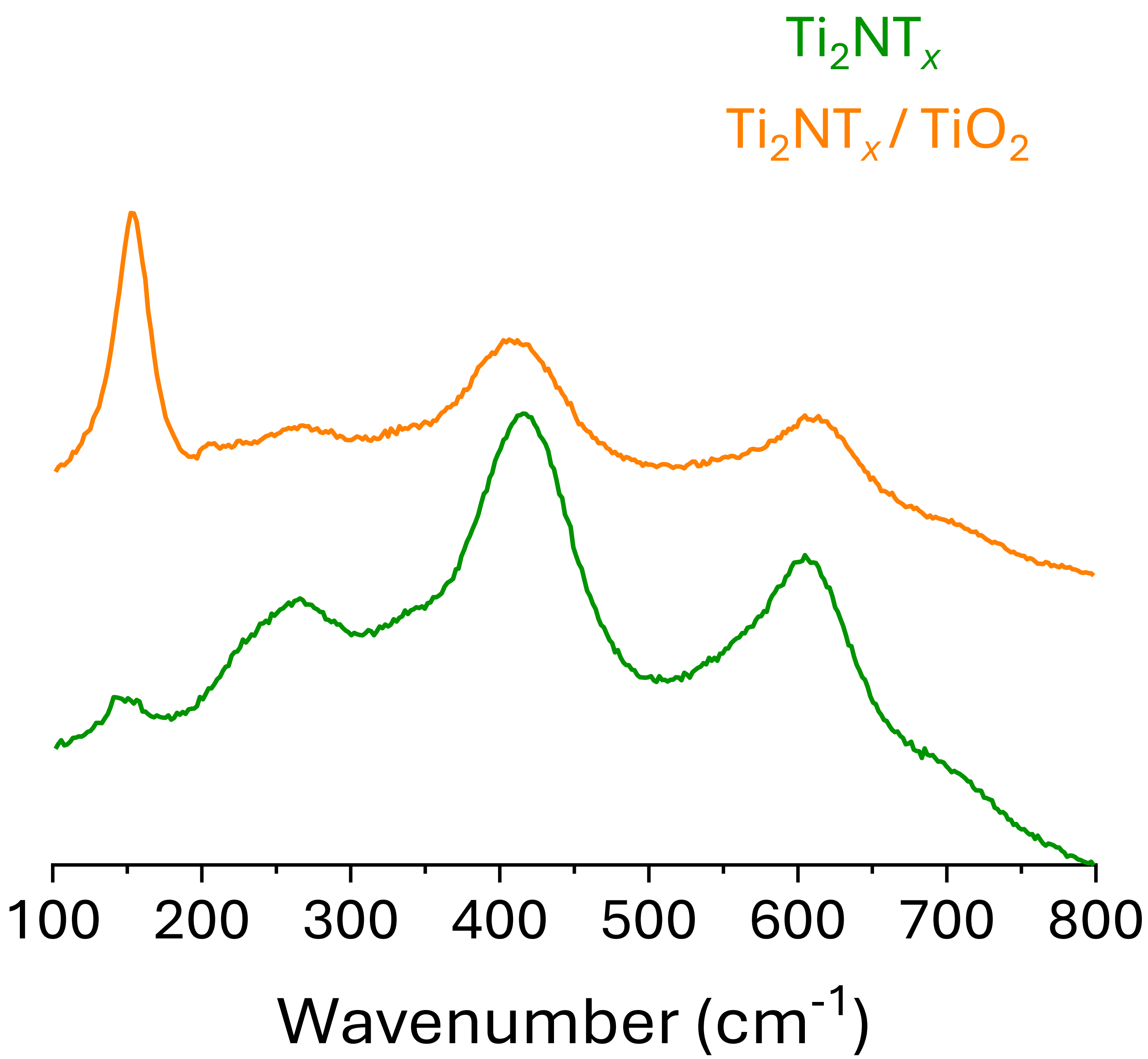
✓ Lattice N atoms are involved in the electrochemical formation of NH_3

❑ Is the formation and replenishment of N vacancies a stable cycle?

Djire et al., J. Am. Chem. Soc. 2025, 147, 29327–29339

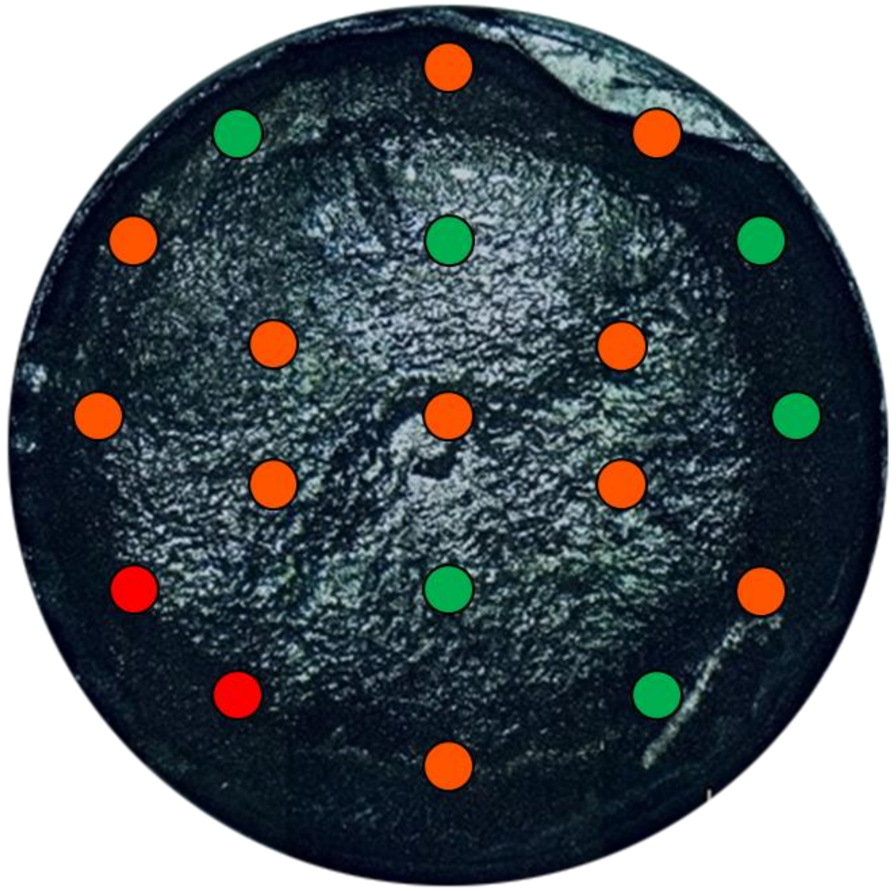
Probing N Replenishment: Before Long-Term NRR

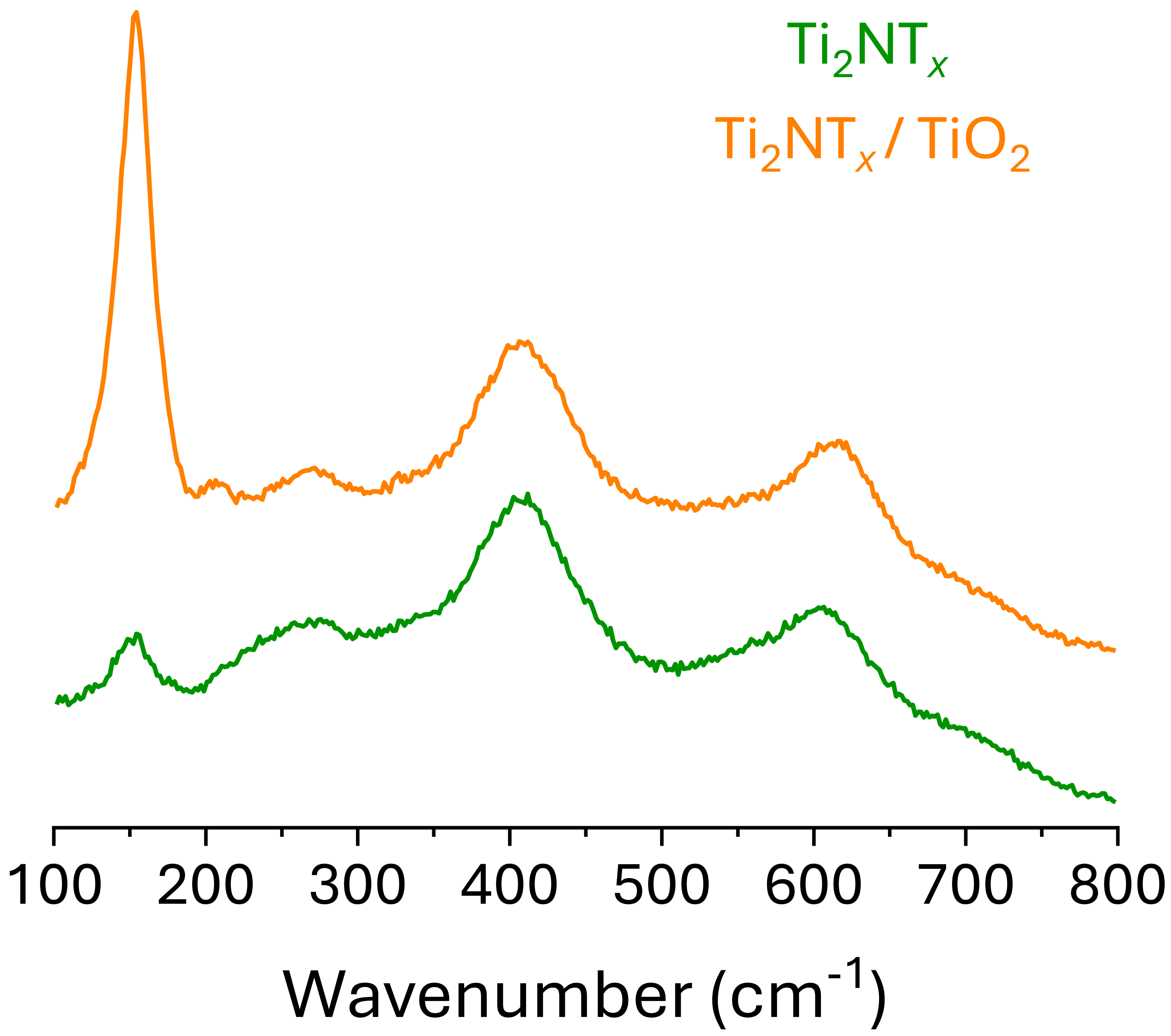




Djire et al., J. Am. Chem. Soc. 2025, 147, 29327–29339

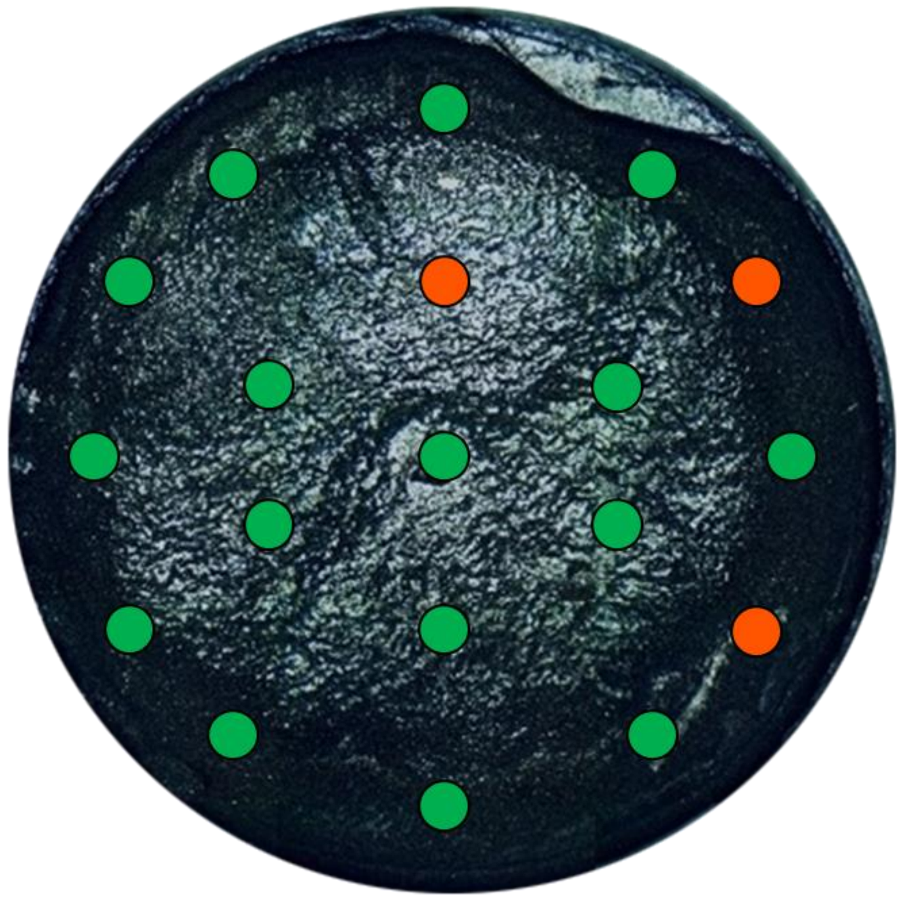
Probing N Replenishment: After Long-Term NRR with Ar

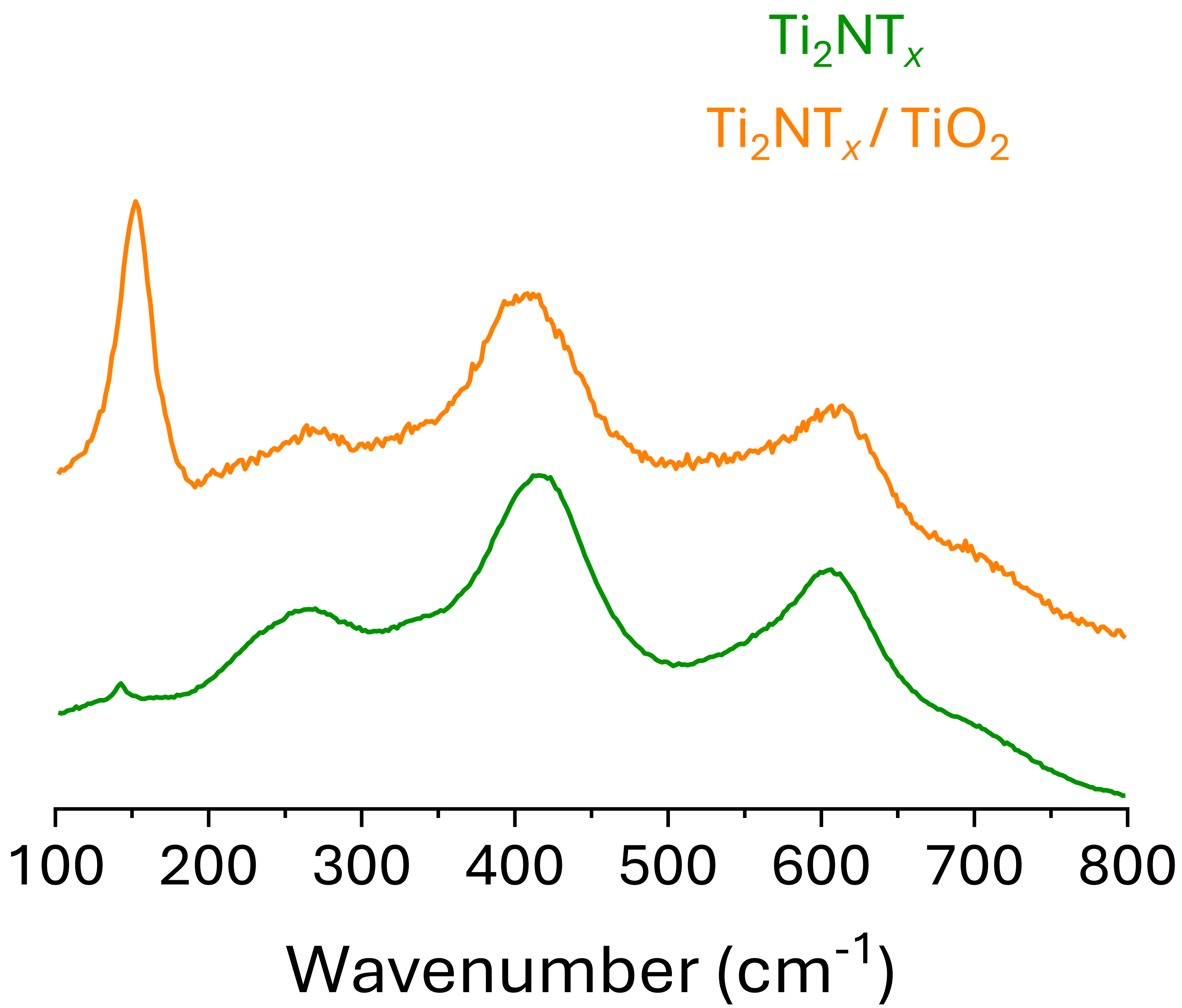




Djire et al., J. Am. Chem. Soc. 2025, 147, 29327–29339

After Long-Term NRR with N_2 as Replenishment





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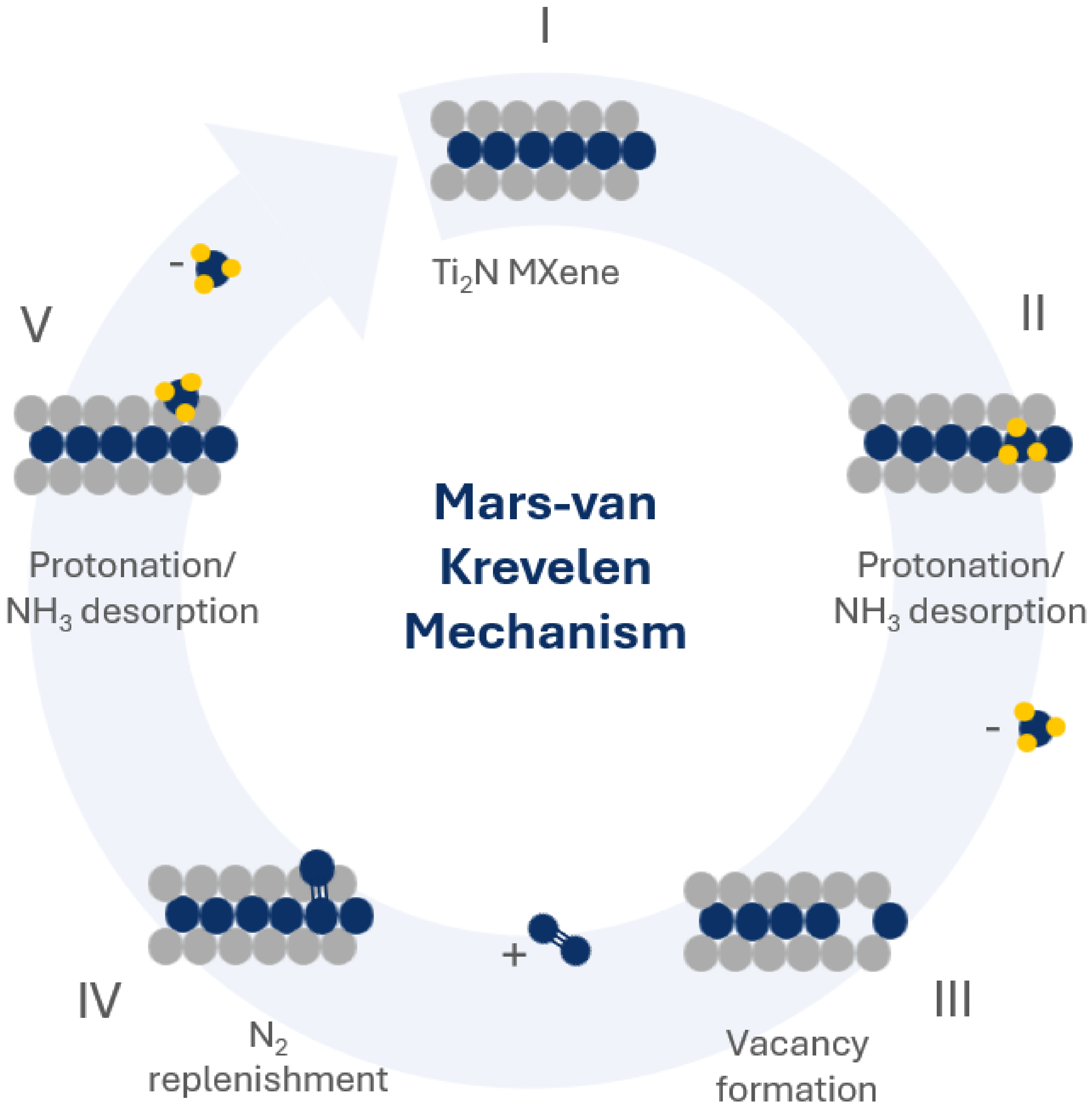
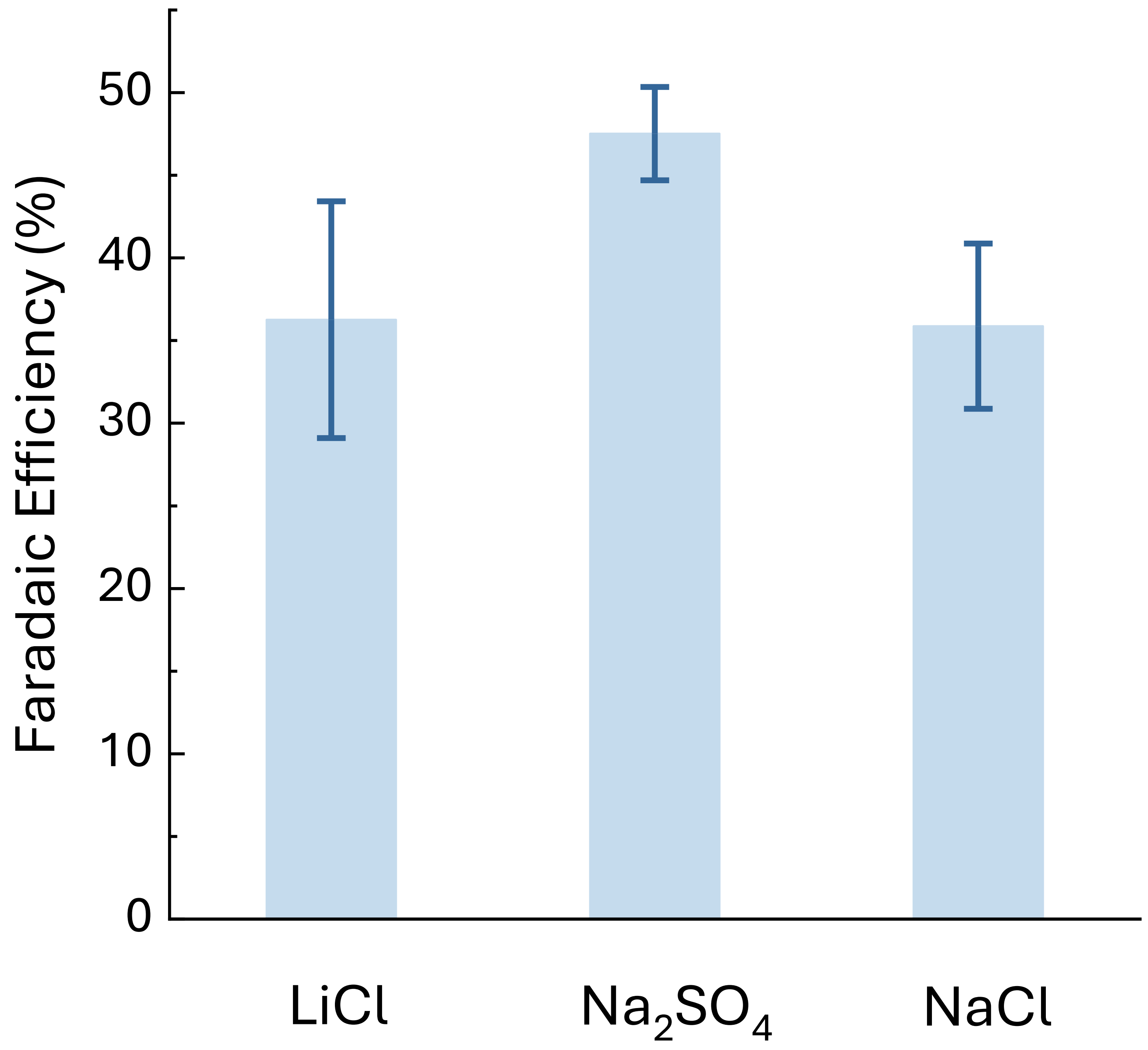
Our Approach of Ammonia Synthesis via MvK Mechanism



- ✓ Lattice N atoms are involved in the electrochemical formation of NH_3
- ✓ The formation and replenishment of N vacancies are a stable cycle

Djire et al., J. Am. Chem. Soc. 2025, 147, 29327–29339

Leveraging MvK to Improve Ammonia Selectivity



MvK mechanism understood and exploited

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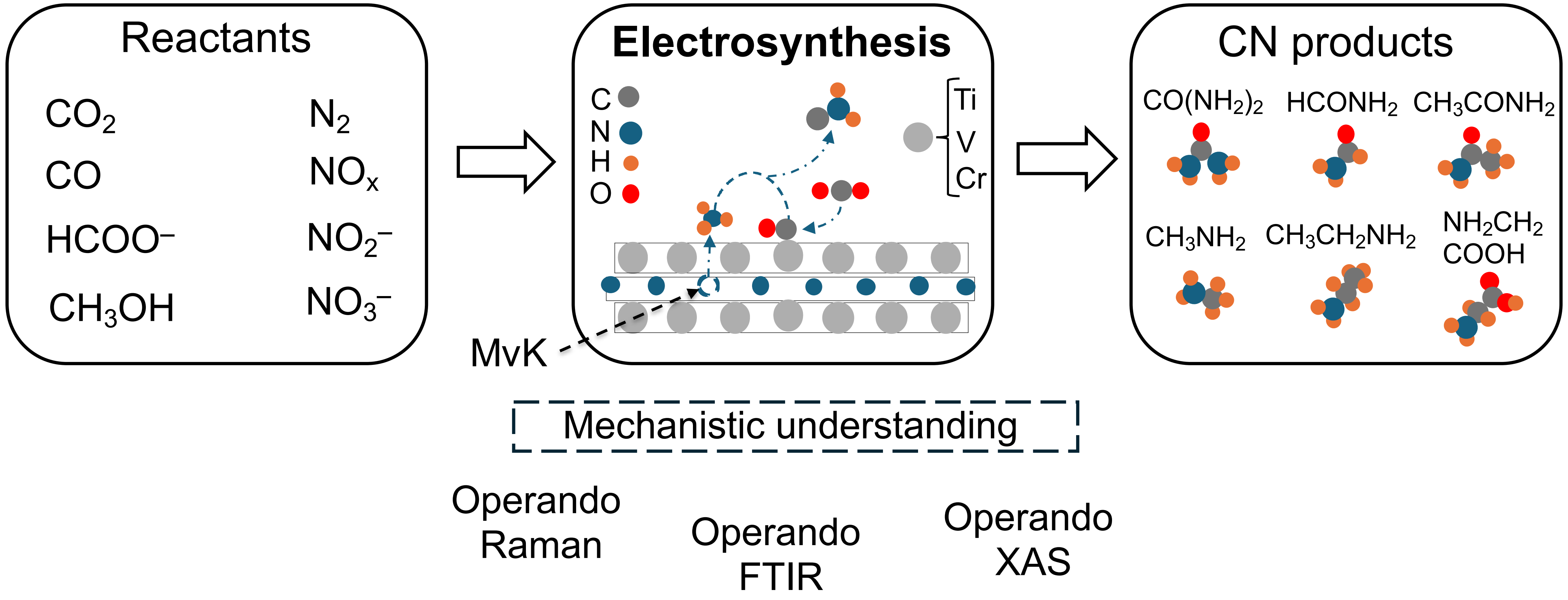
Beyond NH_3: C-C and C-N Coupling with MNenes



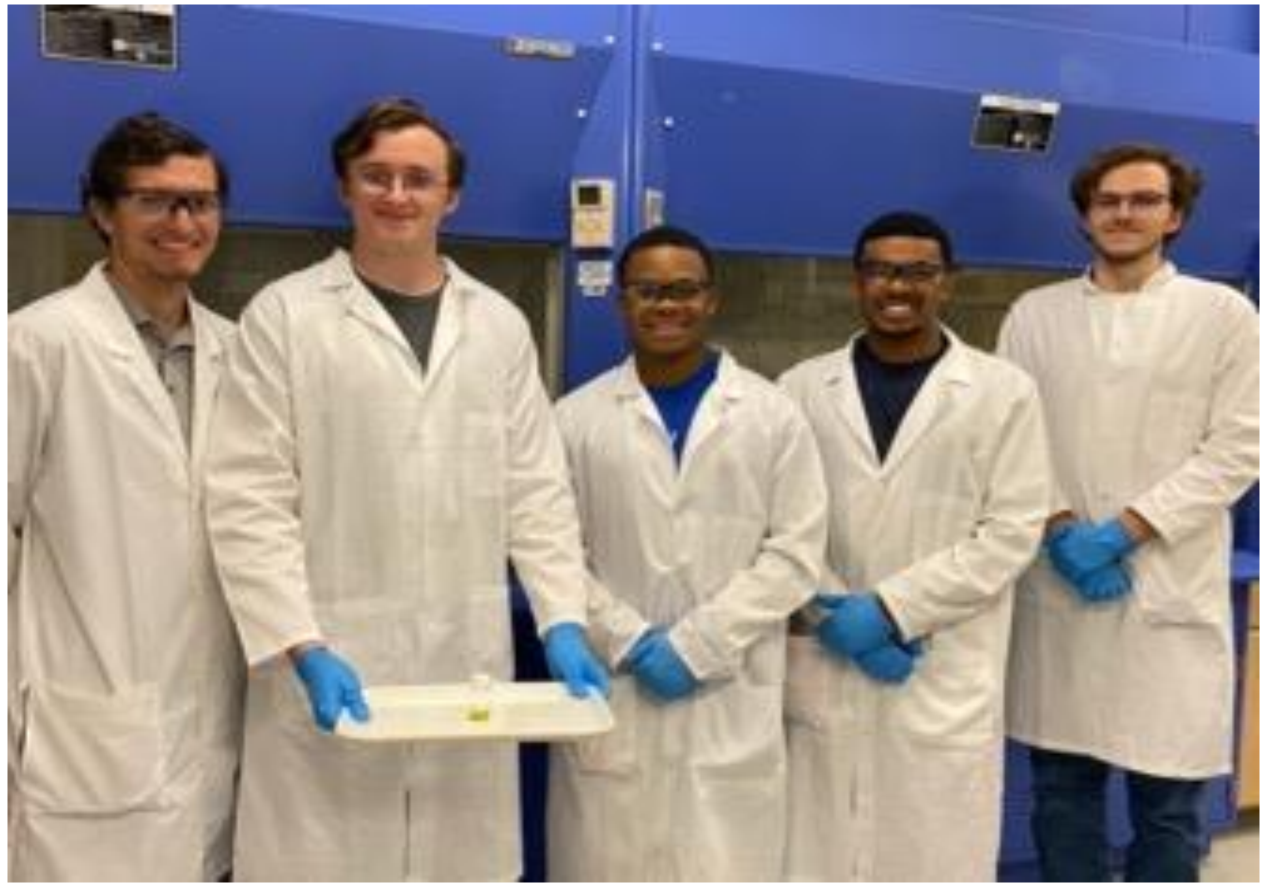
We will exploit MvK in NH_3, C-C and C-N coupling chemistries by investigating MNenes with various M combinations, C-N ratios, and terminal groups

- Perform electrochemical reactions
- NMR and GC-MS to reveal liquid and gas products
- Operando spectroelectrochemical analyses to understand mechanisms

Acknowledgements

DJIRE Group

DJIRE URM Summer Program



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