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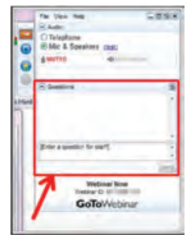

Type them into questions box!

"Why am I muted?"
Don't worry. Everyone is muted except the presenter and host. Thank you and enjoy the show.

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Culinary Chemistry

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Why does food taste better when it is grilled or what molecular compounds make a great wine? Discover the delectable science of your favorite food and drink and don't forget to come back for a second helping.

Popular Chemistry

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Feeling burdened by all that molecular weight? Listen to experts expound on the amazing side of current hot science topics. Discover the chemistry of rockets, how viruses have affected human history, or the molecular breakdown of a hangover.

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Learn from the best and brightest minds in chemistry! Hundreds of webinars on diverse topics presented by experts in the chemical sciences and enterprise.

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ACS Office of Philanthropy
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A Career Planning Tool For Chemical Scientists

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https://chemidp.acs.org

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We believe in the strength of diversity in all its forms, because inclusion of and respect for diverse people, experiences, and ideas lead to superior solutions to world challenges and advances chemistry as a global, multidisciplinary science.

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ACS Committee on Science (COMSCI)

"The ACS Committee on Science aims to ***engage the global chemistry enterprise to build a better tomorrow*** by identifying new frontiers of chemistry, examining the scientific basis of, and formulate public policies related to, the chemical sciences, and recognizing outstanding chemical scientists."

https://www.acs.org/content/acs/en/about/governance/committees/science.html

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ACS
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Chemistry on Capitol Hill
2021 Emerging Policies

Date: Wednesday, June 30, 2021 @ 2-3pm ET
Speakers: Caroline Trupp Gil, American Chemical Society / Karen Garcia, American Chemical Society / Carl Maxwell, American Chemical Society
Moderator: Lauren Posey, American Chemical Society

Register for Free!

What You Will Learn:

- How the Biden Administration and 117th Congress are shaping up in terms of its STEM priorities
- Which specific pieces of legislation or federal policies will be likely to impact ACS members
- How members can become involved

Co-produced with: ACS Government Affairs

Designing Bio-Sourced Polymers
that Enable Recycling

Date: Thursday, July 1, 2021 @ 2-3pm ET
Speaker: Stefan Mecking, University of Konstanz
Moderator: Mark Jones, Dow Chemical (retired)

Register for Free!

What You Will Learn:

- What is solvolysis and how it can enable plastics recycling
- How renewable polycarbonates and polyesters with a low density of in-chain functional groups as break points in a polyethylene chain can be recycled chemically
- How long-chain building blocks for polycondensation can be created from common plant oil feedstocks or microalgae oils

Co-produced with: ACS Division of Polymer Chemistry

Succeeding in a Global Environment
Successfully Working Across Cultures

Date: Wednesday, July 7, 2021 @ 2-3pm ET
Speaker: Ramki Subramnian, DowAksa USA
Moderator: Tom Halleran, American Chemical Society

Register for Free!

What You Will Learn:

- Why there are many aspects to culture and what are some of the many similarities & differences across those aspects
- Why your ability to work effectively across cultures is an important contributor to success
- How your overall career is a marathon, but the environment can change rapidly, requiring you to constantly observe and adapt to the culture around you

Co-produced with: ACS Careers

www.acs.org/acswebinars

ACS
Chemistry for Life®

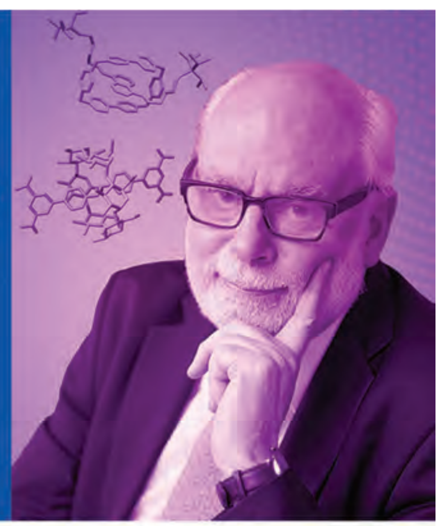
ACS President
H.N. Cheng Presents: FRONTIER FRIDAYS

co-produced with the ACS Committee on Science

Artificial Molecular Machines

Going from Solution to Surfaces

Featuring 2016 Nobel Laureate in Chemistry **Sir Fraser Stoddart**



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THIS ACS WEBINAR WILL BEGIN SHORTLY...

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ACS Chemistry for Life®

Artificial Molecular Machines: Going from Solution to Surfaces

SIR FRASER STODDART
2016 Nobel Laureate in Chemistry, Board of Trustees Professor of Chemistry, Northwestern University

H.N. CHENG
President, American Chemical Society

YOUNG-SHIN JUN
Professor, Depart. of Energy, Environmental & Chemical Engineering, Washington University in St. Louis

Presentation slides are available now! The edited recording will be made available as soon as possible.

www.acs.org/acswebinars

This ACS Webinar is co-produced with the ACS Committee on Science.

Presidential Theme – Growth, Collaboration and Advocacy

ACS Chemistry for Life®

- **Chemistry is a central science.** A strong and growing global chemistry enterprise is good for the profession and its members
- **Some possible actions:**
  - Innovation, new frontiers, new applications
    - Entrepreneurship, industrial engagement
  - Sustainability and green chemistry
  - International partnership and mutual assistance
  - Collaboration
- **Need continued public and government support**

New Frontiers and Opportunities for Chemistry

- Chemistry continues to be a productive field, with new or expanded areas where future chemists and chemical engineers can find exciting opportunities
- Chemistry is also becoming multidisciplinary, and many innovations are found at the interfaces of two or more disciplines
- The goal of the Presidential – Committee on Science Webinar Series and Symposium is to highlight some of the major growth and emerging areas of chemistry, to provide the opportunity to meet the foremost leaders in these areas, and to inform our members and students as to the future directions of chemistry
- Thanks are due to Sir Fraser Stoddart, ACS Committee on Science (particularly Young-Shin Jun, Michael Morello, Martin Kociolek, and Mary Kirchhoff) and the ACS webinar team for their critical role in making these webinars possible.

New Frontiers and Opportunities for Chemistry

ACS New Frontiers Symposium at ACS National Meeting on August 22-24

35 speakers in **9** sessions (all virtual) covering advanced materials, catalysis, nanotechnology, biotechnology, biomedical, electronics, environmental chemistry, advanced food technology, and sustainability.

The first session will start on **Sunday, August 22, at 2:00pm EDT**, and will run continuously until Tuesday, **August 24 at 6:30pm EDT.**

New Frontiers and Opportunities for Chemistry

ACS **"Frontier Friday"** Webinars in May and June

5/28/2021: **Dr. Zhenan Bao**, Stanford University,
"Skin-Inspired Organic Electronics"

6/11/2021: **Dr. Amy Prieto**, Colorado State University,
"Lithium-ion Batteries: The Road to Sustainable Energy Storage"

6/25/2021: **Sir Fraser Stoddart**, Northwestern University,
"Artificial Molecular Machines: Going from Solution to Surfaces"

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Sir Fraser Stoddart, Featured Speaker

- B.Sc. (1964) and Ph.D. (1967) Univ. of Edinburgh; NRCC postdoc at Queen's Univ. (1967-1970)
- University of Sheffield and ICI Corporate Lab, 1970 – 1990.
- Univ. of Birmingham (1990-1997); UCLA (1997-2008) Saul Winstein Professor of Chemistry; Director of California NanoSystems Institute (2002-2008), Kavli Chair of NanoSystems Sciences; Northwestern Univ (since 2008), Board of Trustees Professor of Chemistry
- In 35 years, nearly 300 PhD students and postdocs have been trained in his labs. He has published over 1000 papers; h-index of 130. He is ranked as one of the world's most cited chemists
- Recipients of numerous awards and recognition, including Nobel Prize in Chemistry (2016), member of NAS (2014), Fellow, American Academy of Arts and Sciences (2012), Honorary Fellow of RSC (2011), Knight Bachelor by HM Queen Elizabeth II (2006), ACS Cope Award (2008), and many others

ACS Chemistry for Life®

ACS President H.N. Cheng Presents: FRONTIER FRIDAYS

co-produced with the ACS Committee on Science

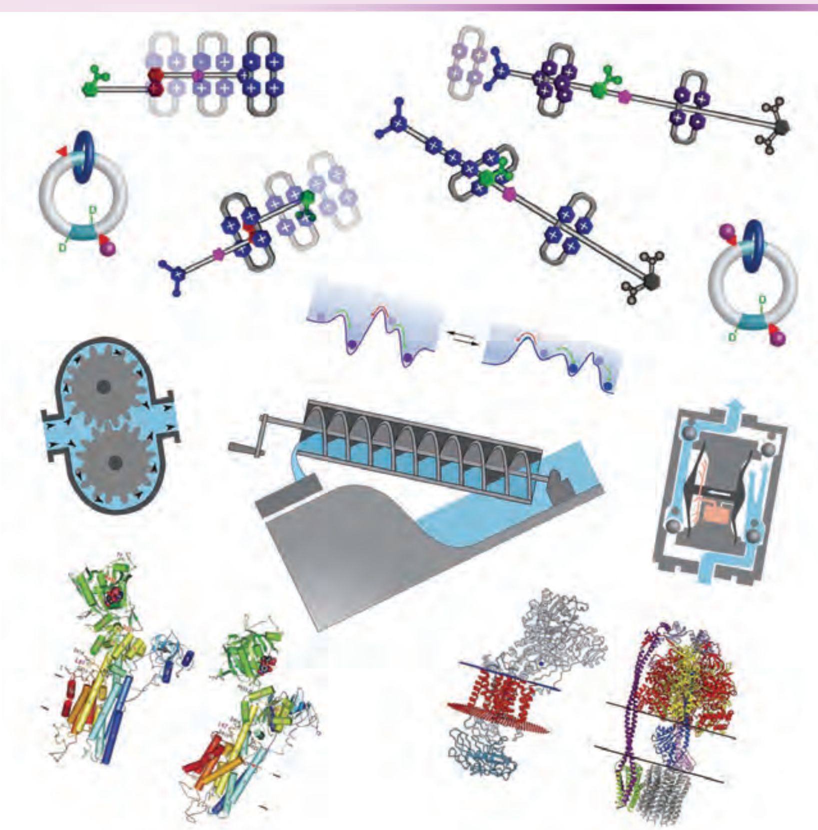
Artificial Molecular Machines

Going from Solution to Surfaces

Featuring 2016 Nobel Laureate in Chemistry **Sir Fraser Stoddart**

The University of Edinburgh · Queen's University · The University Of Sheffield. · ICI · University of Birmingham · UCLA · Northwestern University · Tianjin University

PUMPS THROUGH THE AGES



Nanoscopic Molecular Pumps

Macroscopic Pumps

Microscopic Biomolecular Pumps

Pumps Through the Ages / *Chem* **2020**, *6*, 1954–1979

Molecular Pumps and Motors / *J. Am. Chem. Soc.* **2021**, *143*, 5569–5591

ACS FRONTIERS FRIDAY ROADMAP

Radical Chemistry | Flashing Energy Ratchets | Away-From-Equilibrium | Mechanisorption

Molecular Pumps Mark I & II → **[3]Catenane Electric Motor** → **Molecular Dual & Duet Pumps** → **Precise Polyrotaxane Synthesizer** → **Robust Dynamics MIMs on MOFs** → **Physisorption Chemisorption Mechanisorption**

Outlook for Molecular Nanotechnology

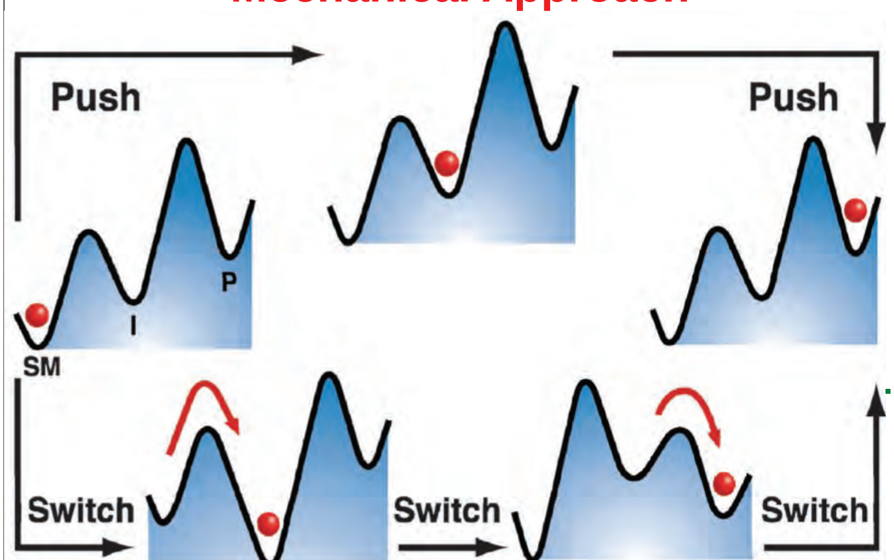
The Rise and Promise of Molecular Nanotopology

Nano Lett. **2020**, *20*, 5597–5600 | *CCS Chem.* **2021**, *3*, 1542–1572

GETTING TO KNOW ARTIFICIAL MOLECULAR MACHINES

Big Machines **"It's Night and Day"** **Small Machines**

Mechanical Approach



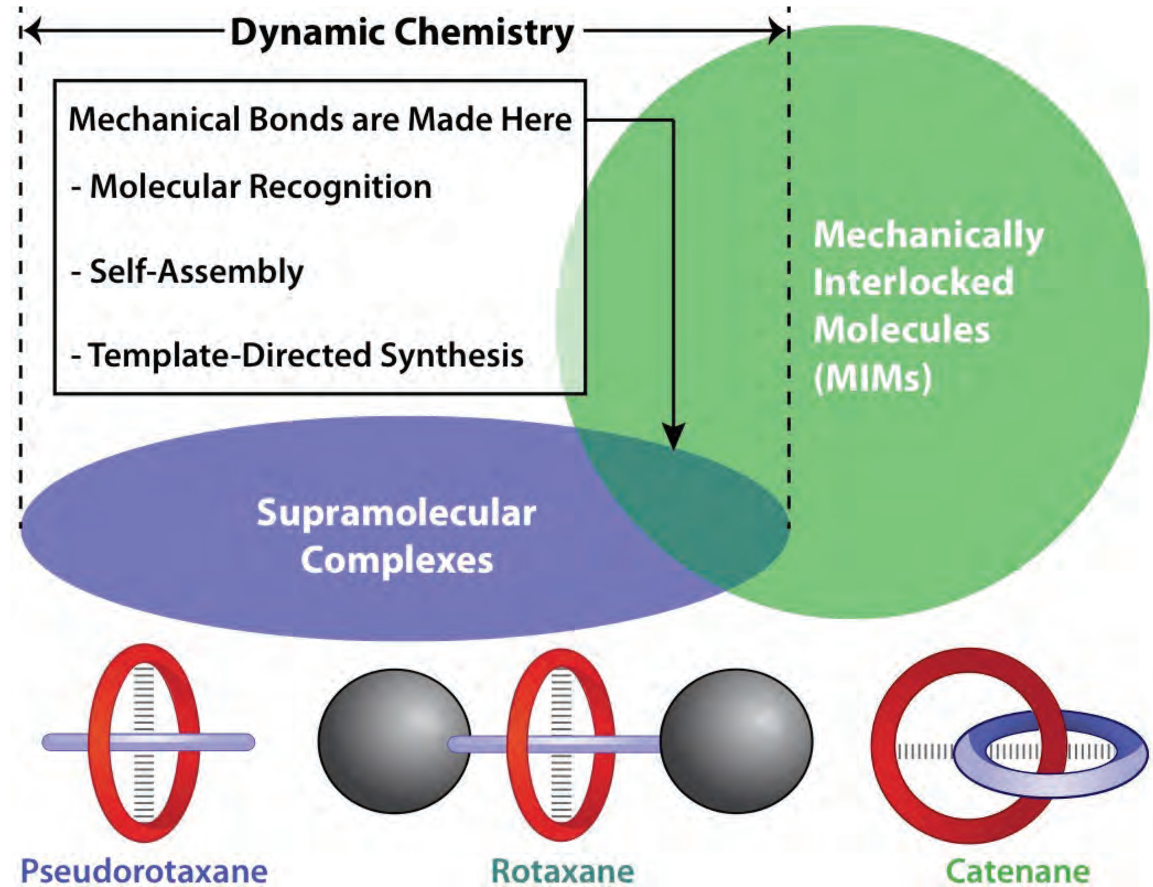
Chemical Approach

Hard to achieve...
...in a top-down manner...
…by mimicking…
…macroscopic machines

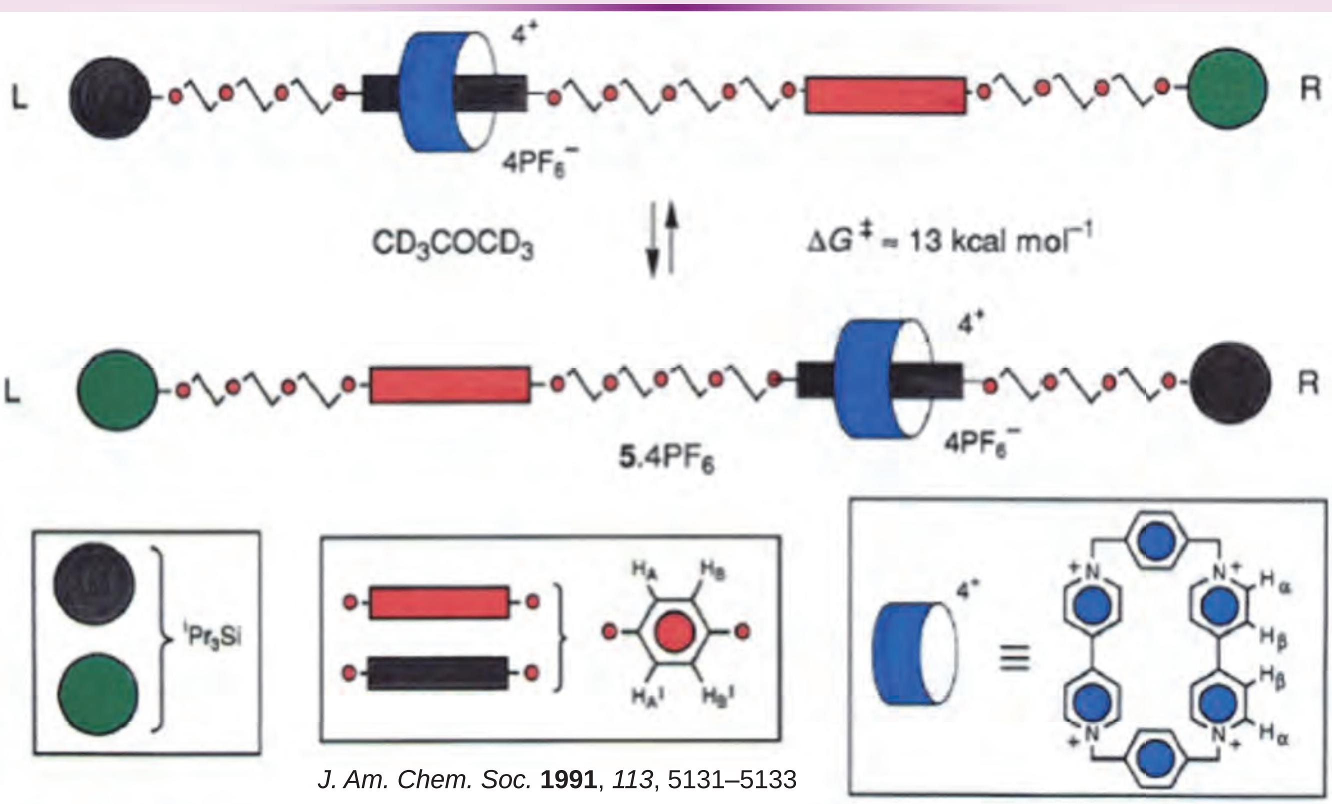
More likely to happen...
...in a bottom-up approach...
…by controlling…
…the free energy states…
…of collections of molecules

"Great Expectations: Can Artificial Molecular Machines Deliver on Their Promise?"
Chem. Soc. Rev. **2012,** *41***,** 19–30

MAKING MECHANICALLY INTERLOCKED MOLECULES (MIMs)



1991 A MOLECULAR SHUTTLE 1991

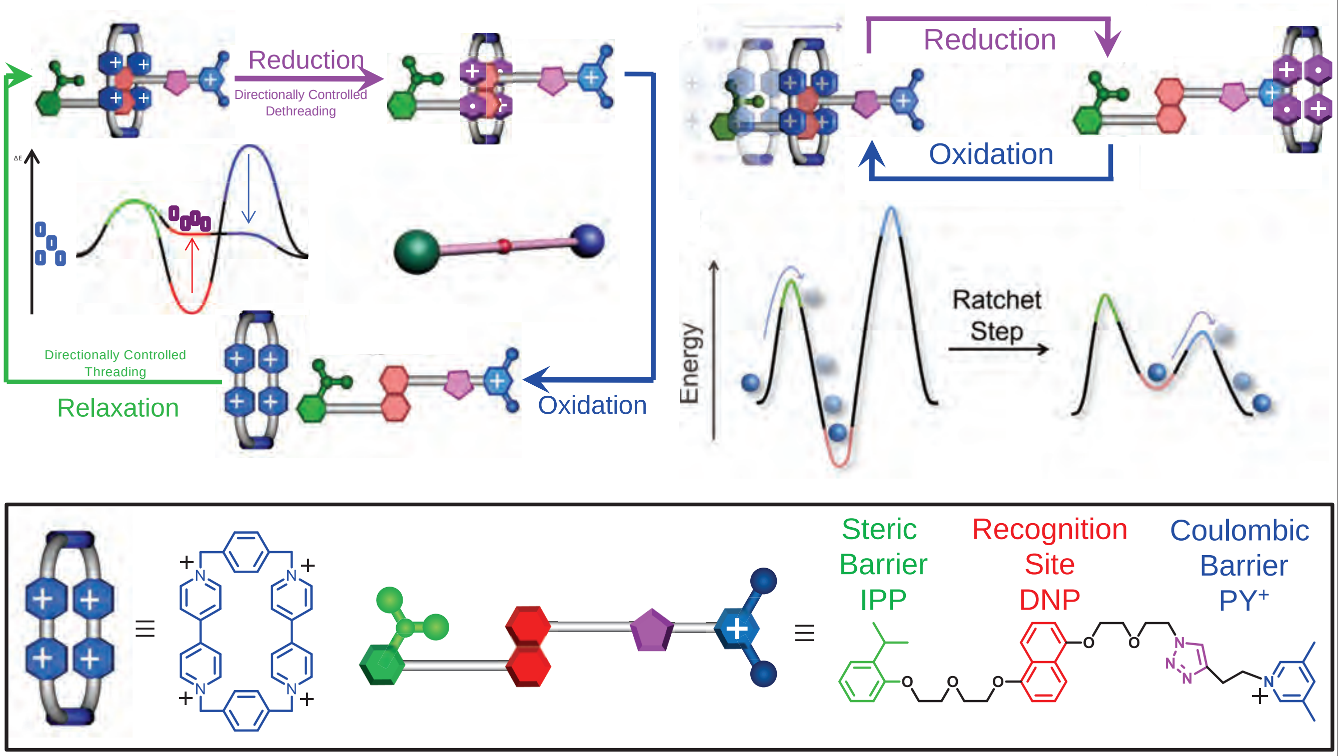


J. Am. Chem. Soc. **1991**, *113*, 5131–5133

Insofar as it becomes possible to control the movement of one molecular component with respect to the other in a [2]rotaxane, the technology for building **molecular machines** will emerge.

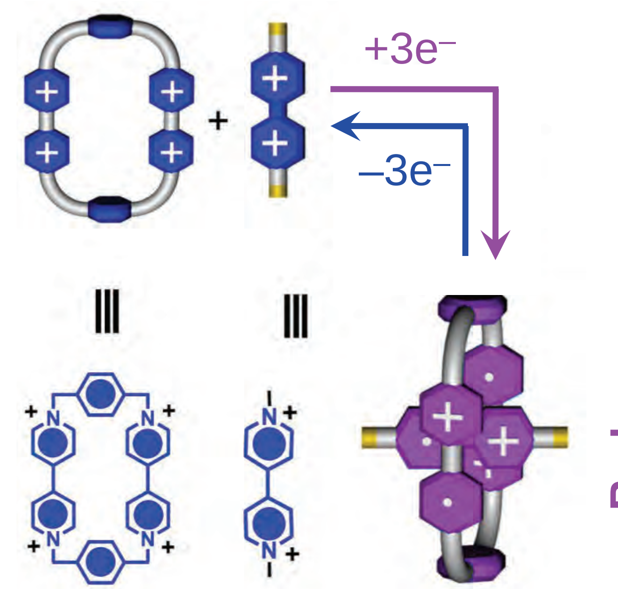
UNIDIRECTIONAL THREADING AND DETHREADING OF A PSEUDOROTAXANE

Flashing Energy Ratchet — Molecular Pump Prototype



J. Am. Chem. Soc. **2013**, *135*, 18609–18620

INTRODUCING RADICALS



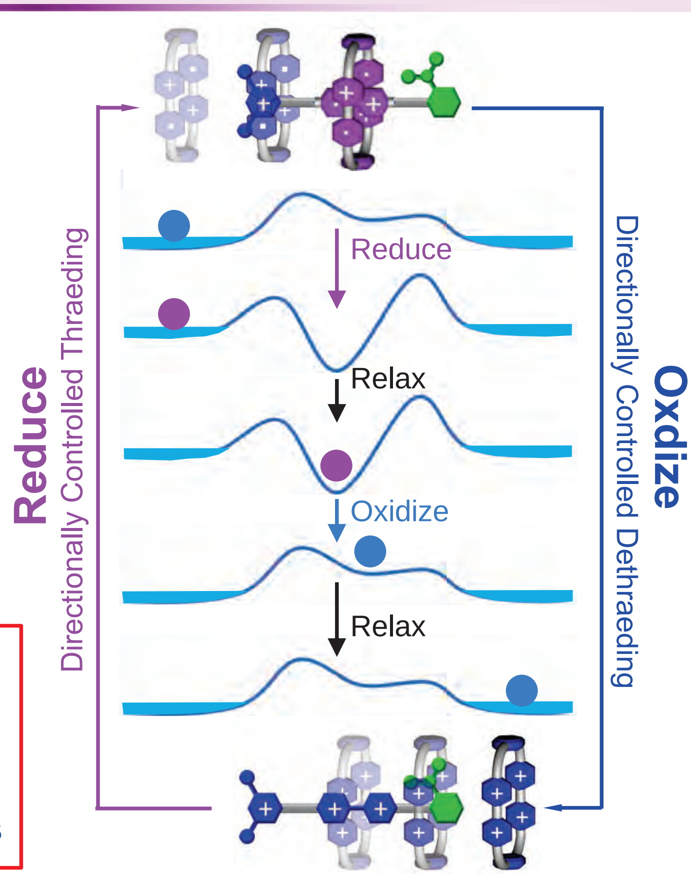
K_a = 50400 M^{-1}

ΔG = – 6.4 kcal mol^{-1}

Attraction under reduced conditions

Repulsion under oxidized conditions

Nature Chem. **2010**, *2*, 42–49



J. Am. Chem. Soc. **2014**, *136*, 14702–14705

KEY FACTORS IN DESIGNING NON-EQUILIBRIUM SYSTEMS

Highly STABILIZING Radical-Radical Interactions

BIPY$^{\bullet+}$ Units |||||||| CBPQT$^{2(\bullet+)}$ Rings

REDUCTION ↑ ↓ **OXIDATION**

BIPY^{2+} Units ((( ))) CBPQT^{4+} Rings

Strongly DESTABILIZING Coulombic Repulsions

⬇

Kinetics of Association and Dissociation
Can be Modulated

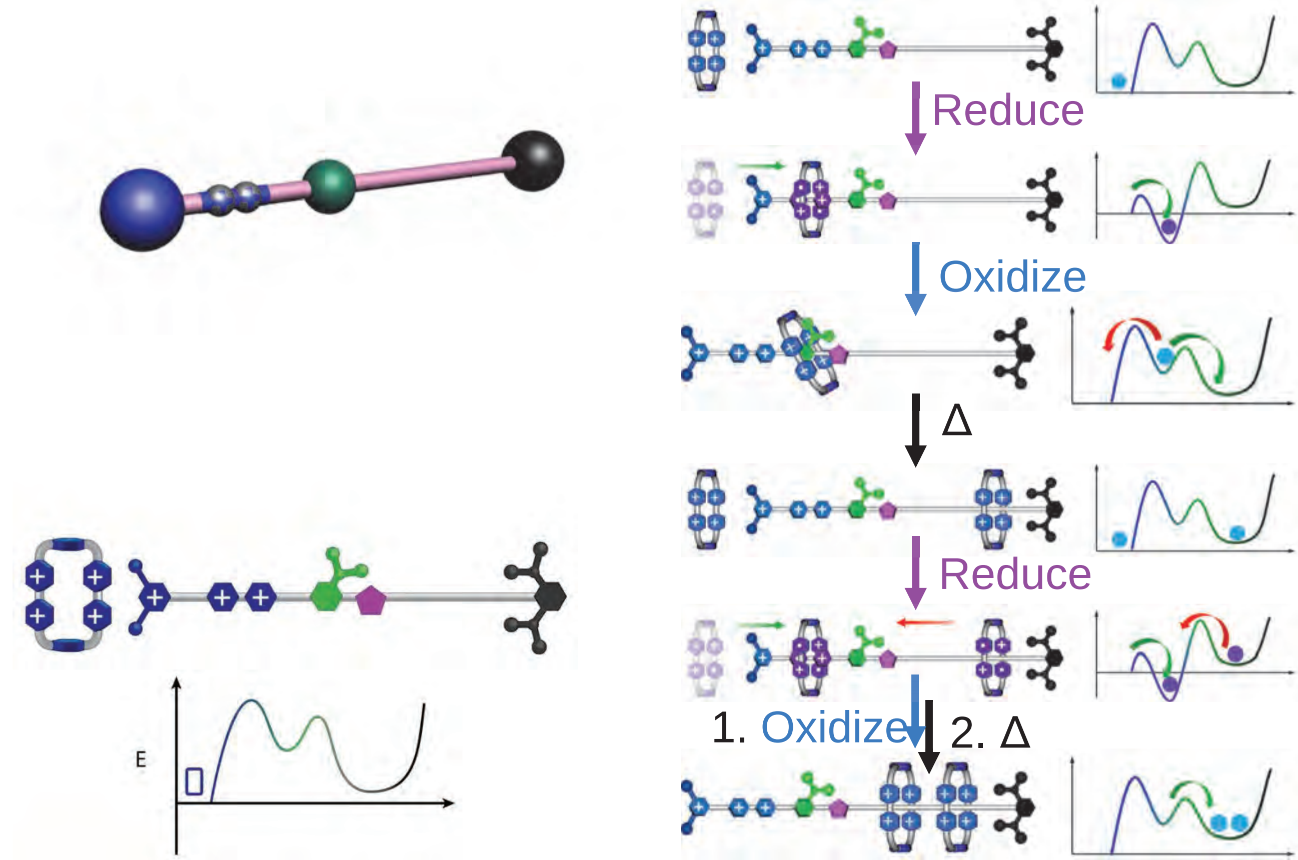
ChemPhysChem **2016**, *17*, 1780–1793

ACS FRONTIERS FRIDAY ROADMAP

Radical Chemistry | Feashing Energy Ratchets | Away-From-Equilibrium | Mechanisorption

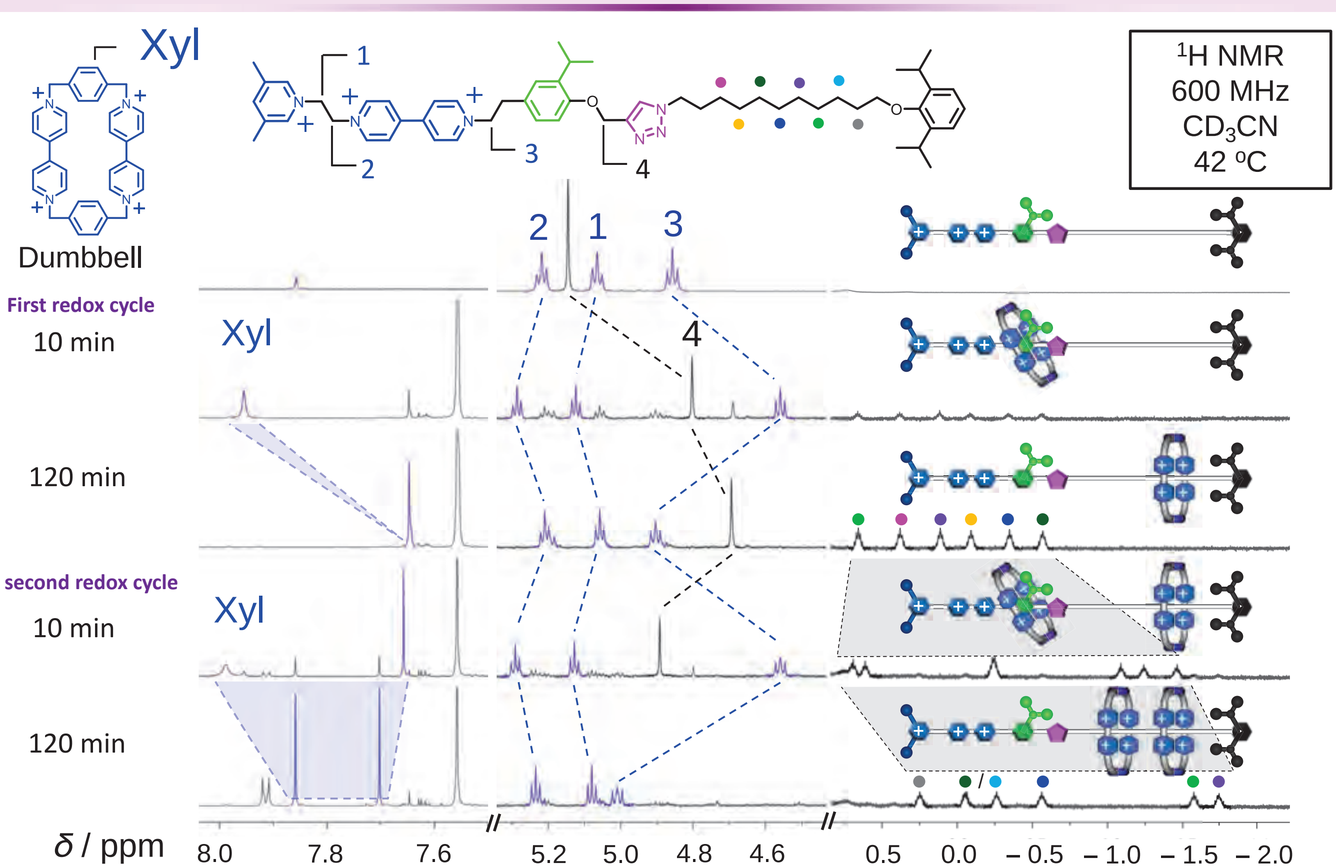
Molecular Pumps Mark I & II

MOLECULAR PUMP DESIGN BLUEPRINT



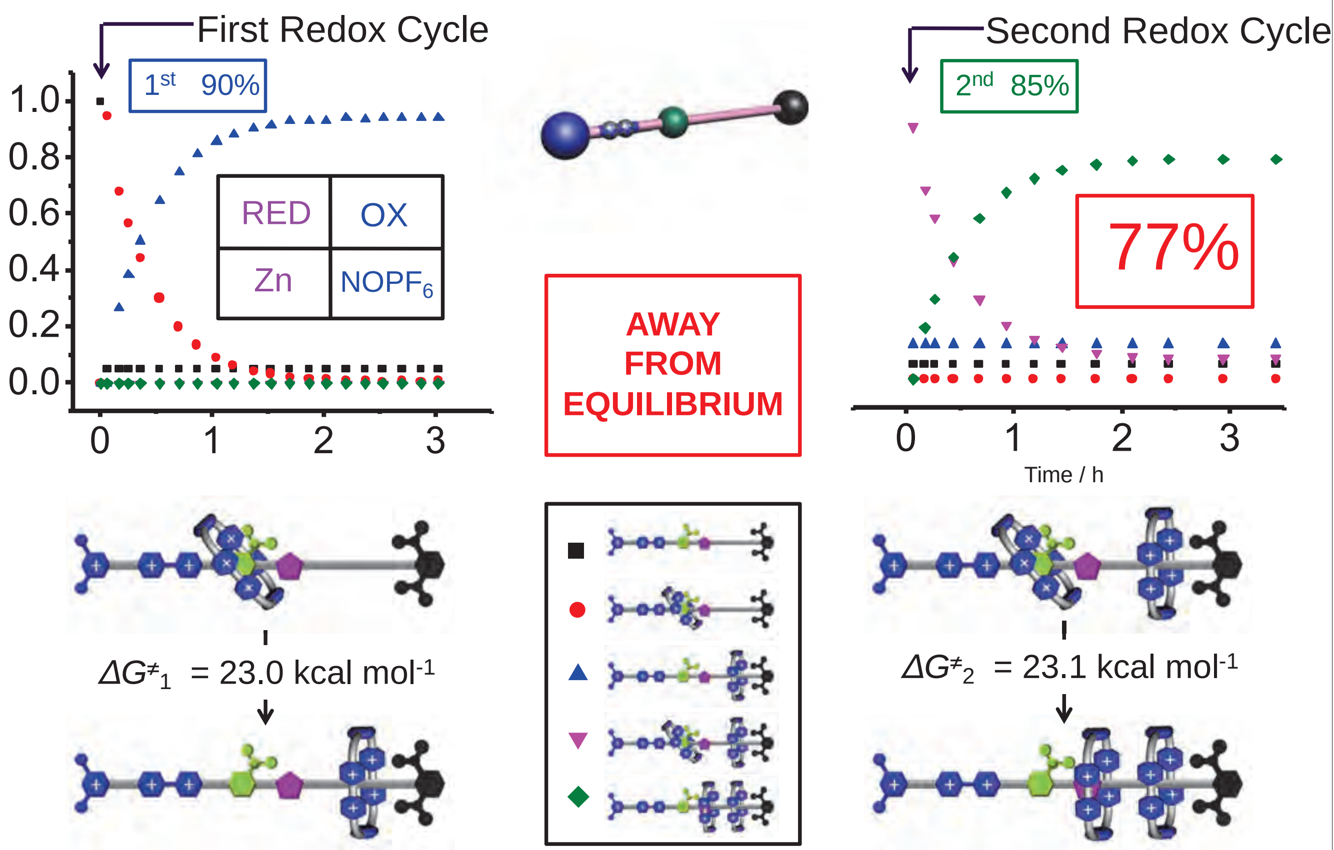
Nature Nanotechnol. **2015**, *10*, 547–553

SYSTEM MOVES AWAY FROM EQUILIBRIUM



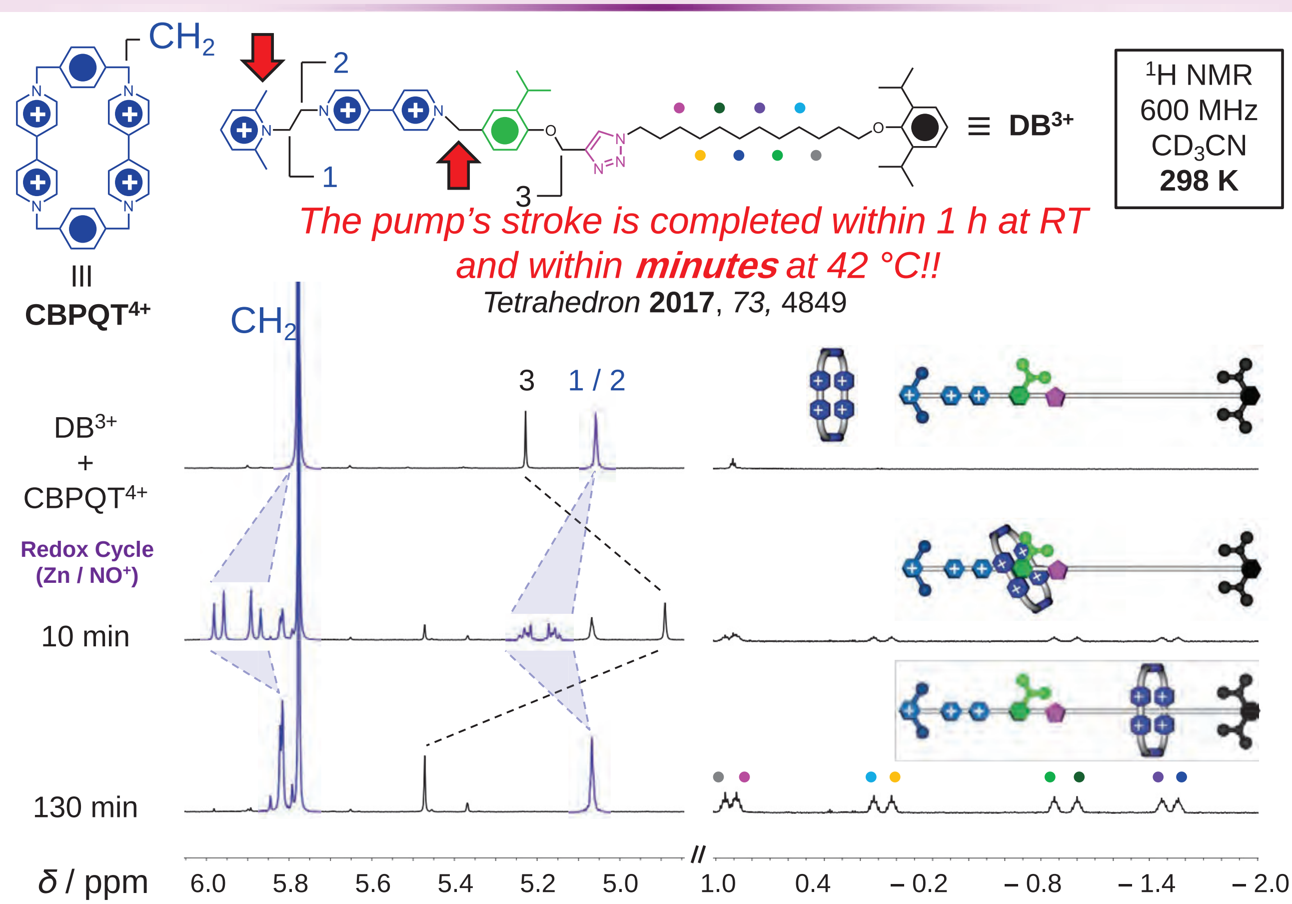
Nature Nanotechnol. **2015**, *10*, 547–553

PUMPING ONE FOLLOWED BY TWO RINGS



Nature Nanotechnol. **2015**, *10*, 547–553

NEW DESIGN | EFFICIENT OPERATION



*The pump's stroke is completed within 1 h at RT and within **minutes** at 42 °C!!*

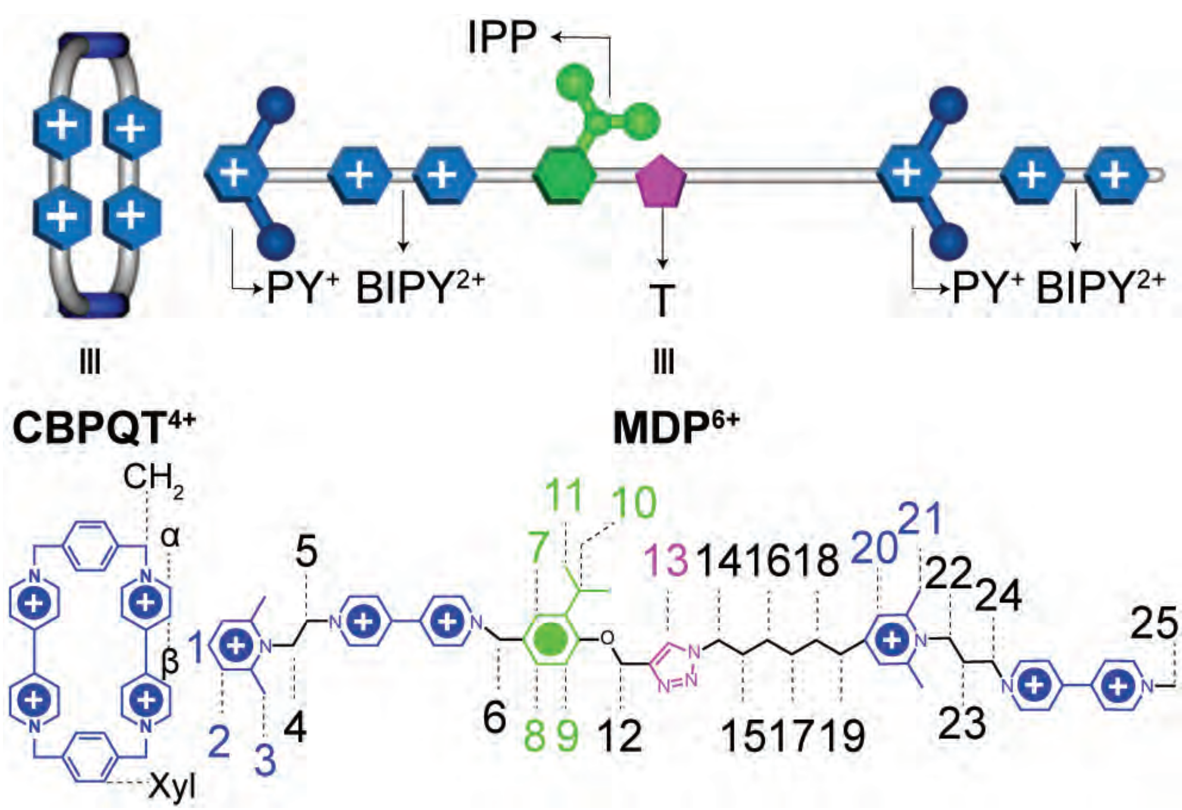
Tetrahedron **2017**, *73,* 4849

ACS FRONTIERS FRIDAY ROADMAP

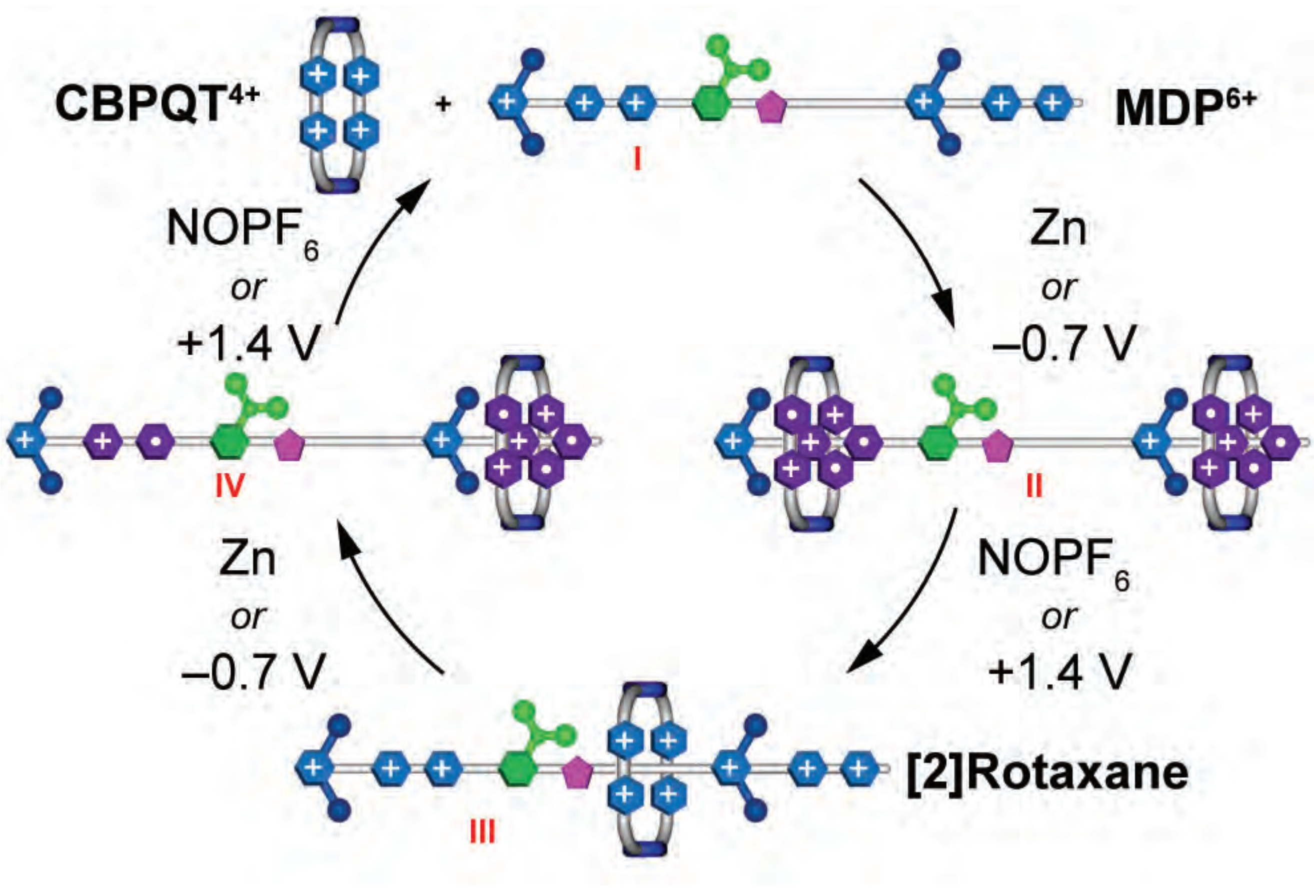
Radical Chemistry | Feashing Energy Ratchets | Away-From-Equilibrium | Mechanisorption

Molecular Pumps Mark I & II → **[3]Catenane Electric Motor** → **Molecular Dual & Duet Pumps**

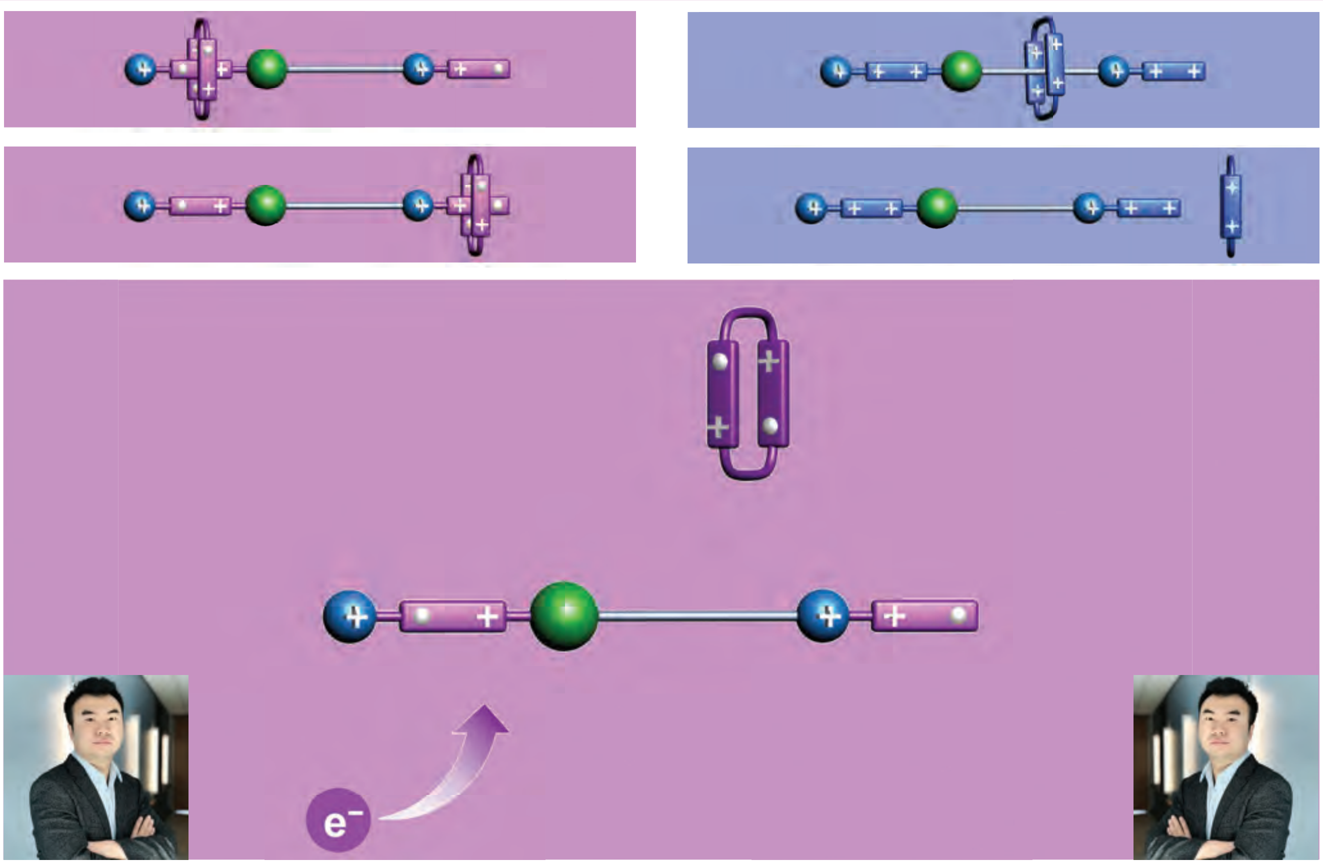
MOLECULAR DUAL PUMP DESIGN



CONTROLLED CAPTURE AND RELEASE PROCESS



2019 MOLECULAR DUAL PUMP 2019

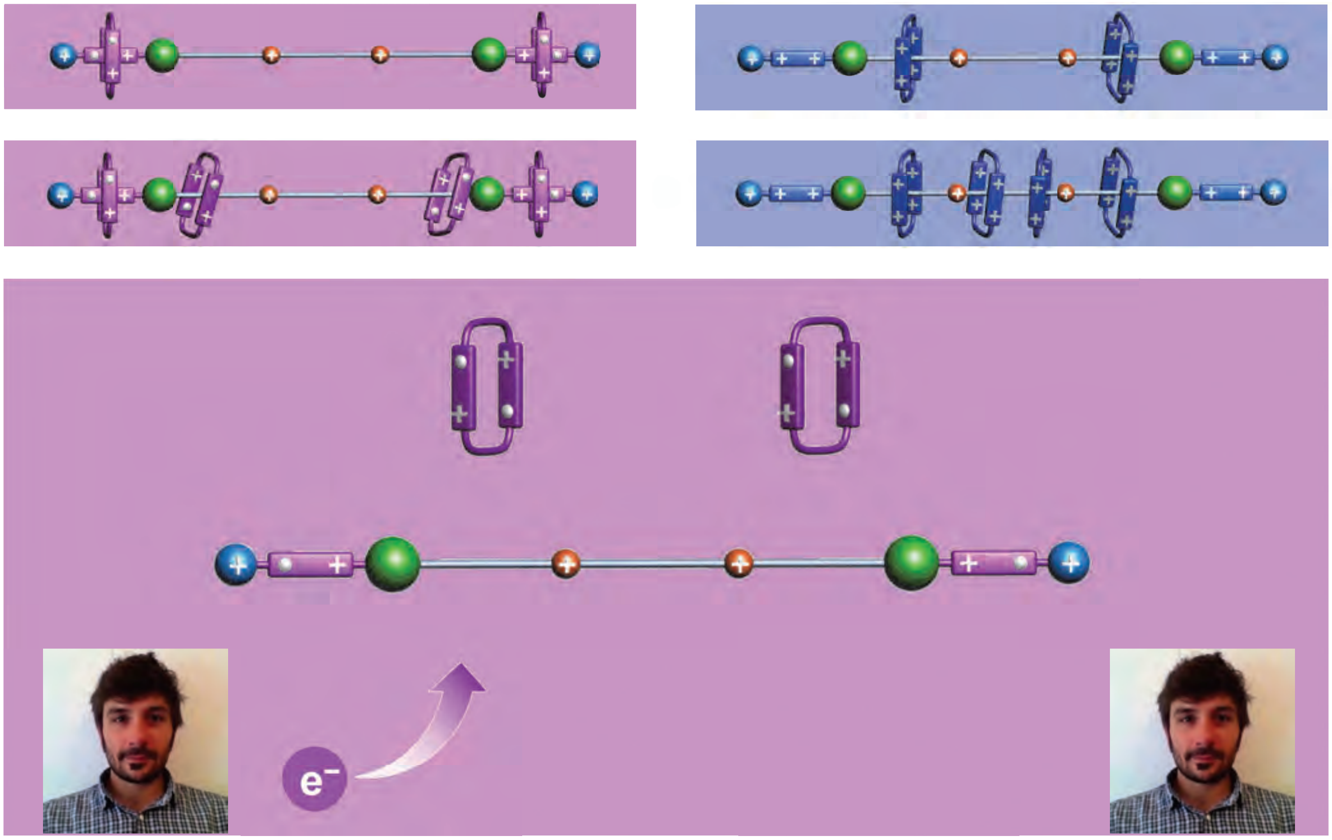


Yunyan Qiu

J. Am. Chem. Soc. **2019**, *141*, 17472−17476

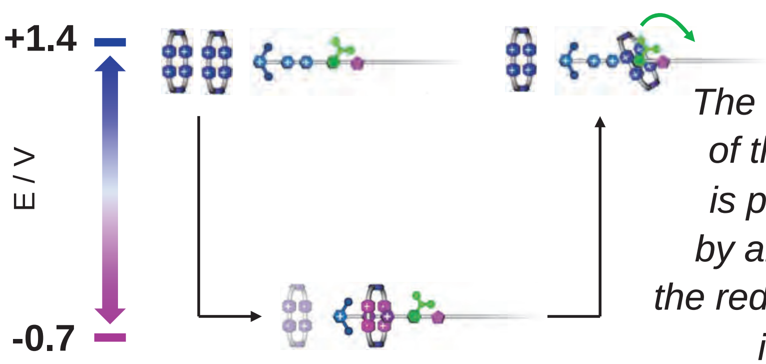
Yunyan Qiu

MOLECULAR DUET PUMP

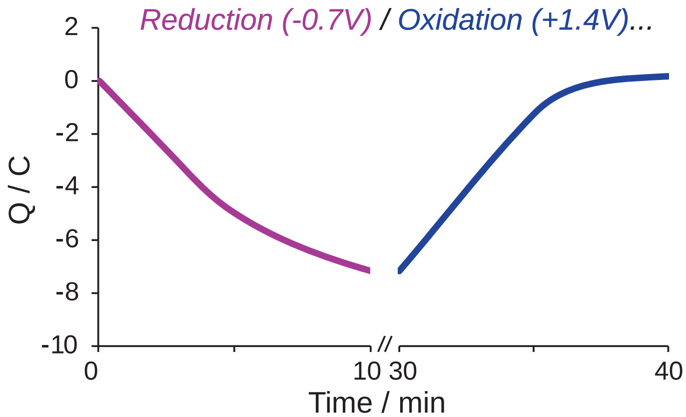


Cristian Pezzato *Angew. Chem. Int. Ed.* **2018**, *57*, 9325–9329 Cristian Pezzato

PUMP OPERATION AND COULOMETRY / 1

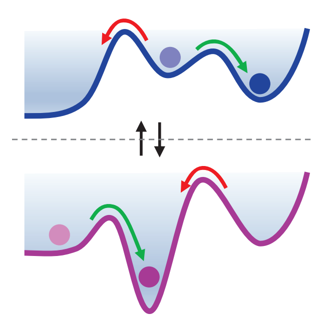


...Coulombs Consumed / Released upon Reduction (-0.7V) / Oxidation (+1.4V)...

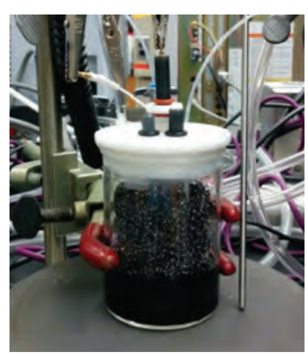


The operation of the pump is promoted by alternating the redox potential in situ

Oxidized State



Reduced State



DP1^{8+} / CBPQT^{4+}

50 : 1000 µM

0.1 M TBAPF$_6$

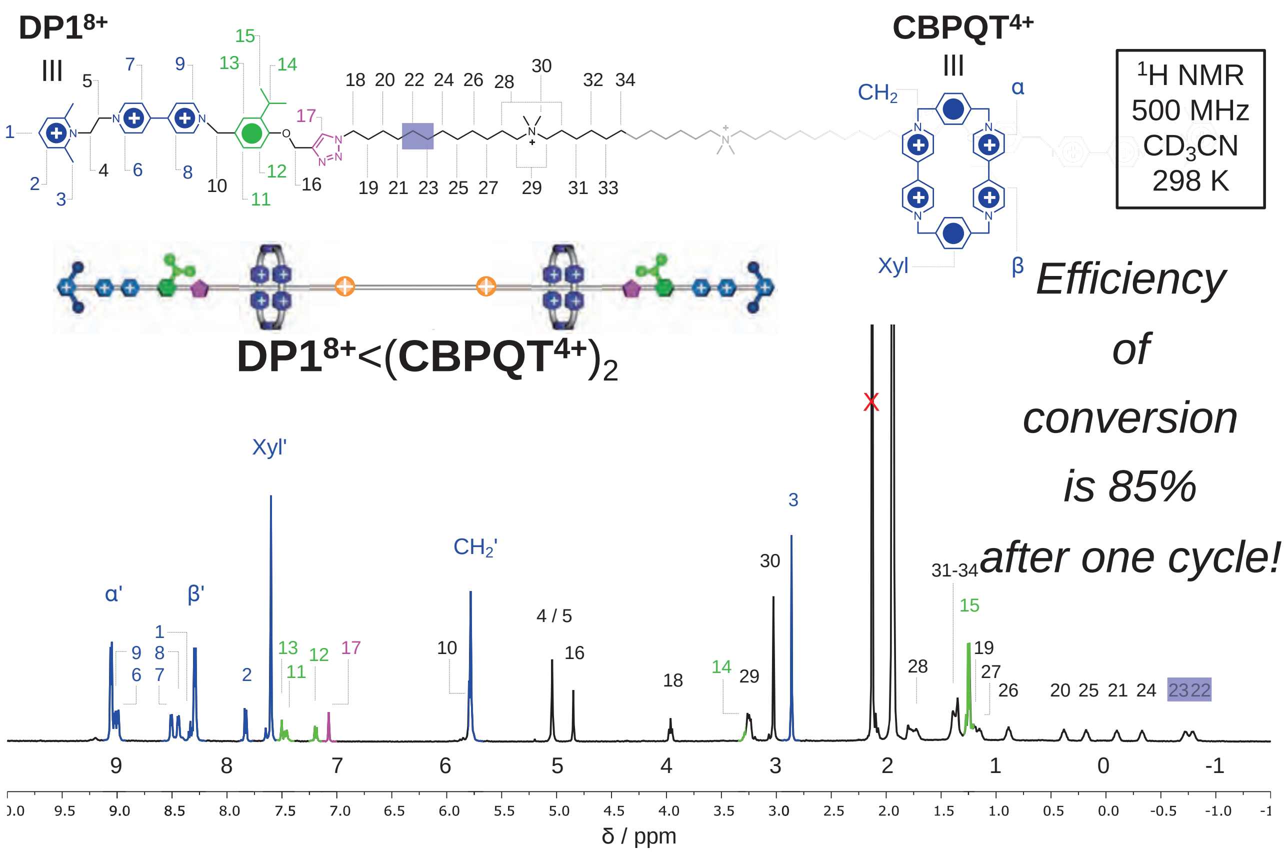
Dry MeCN

313 K

Bulk Electrolysis Setup & Conditions

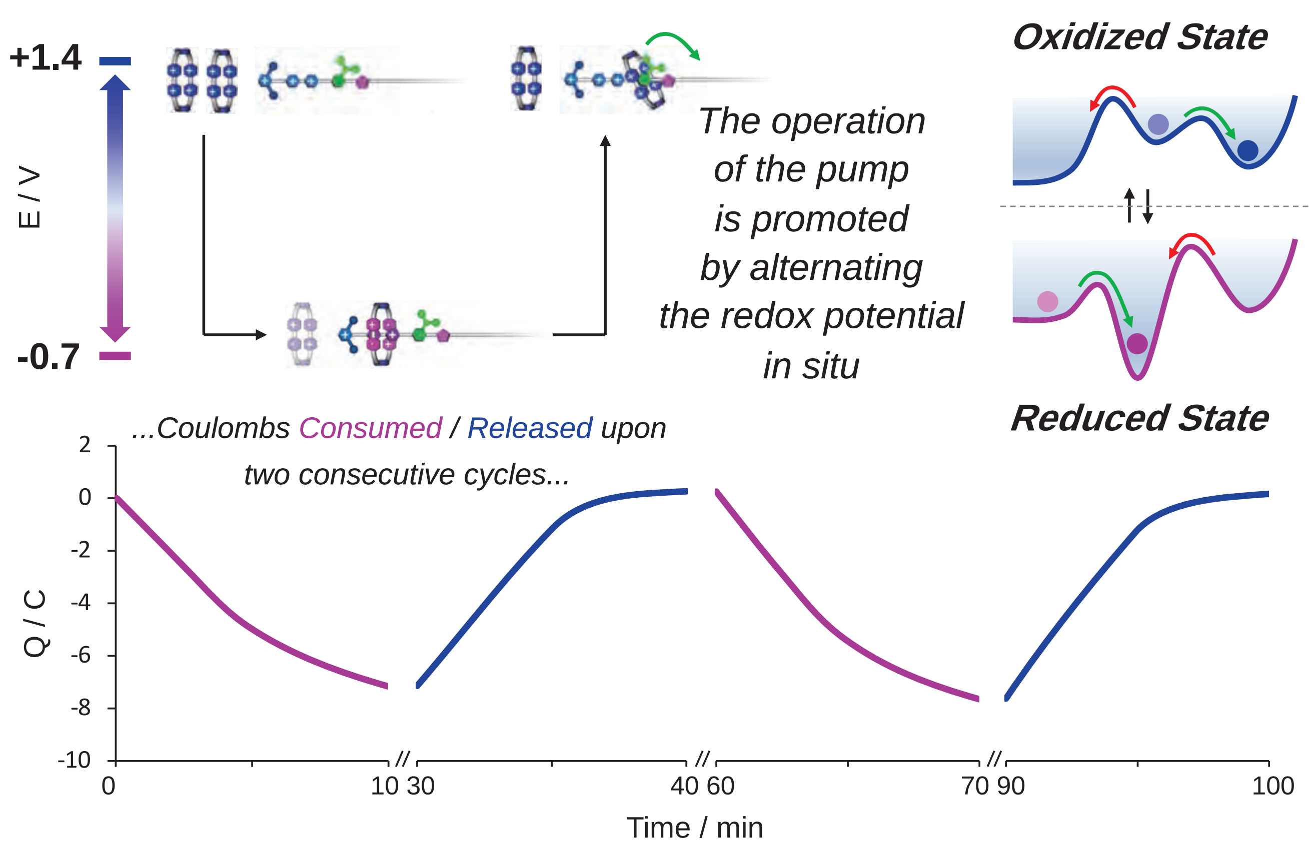
Angew. Chem. Int. Ed. **2018**, *57*, 9325–9329

AFTER ONE CYCLE / [3]ROTAXANE



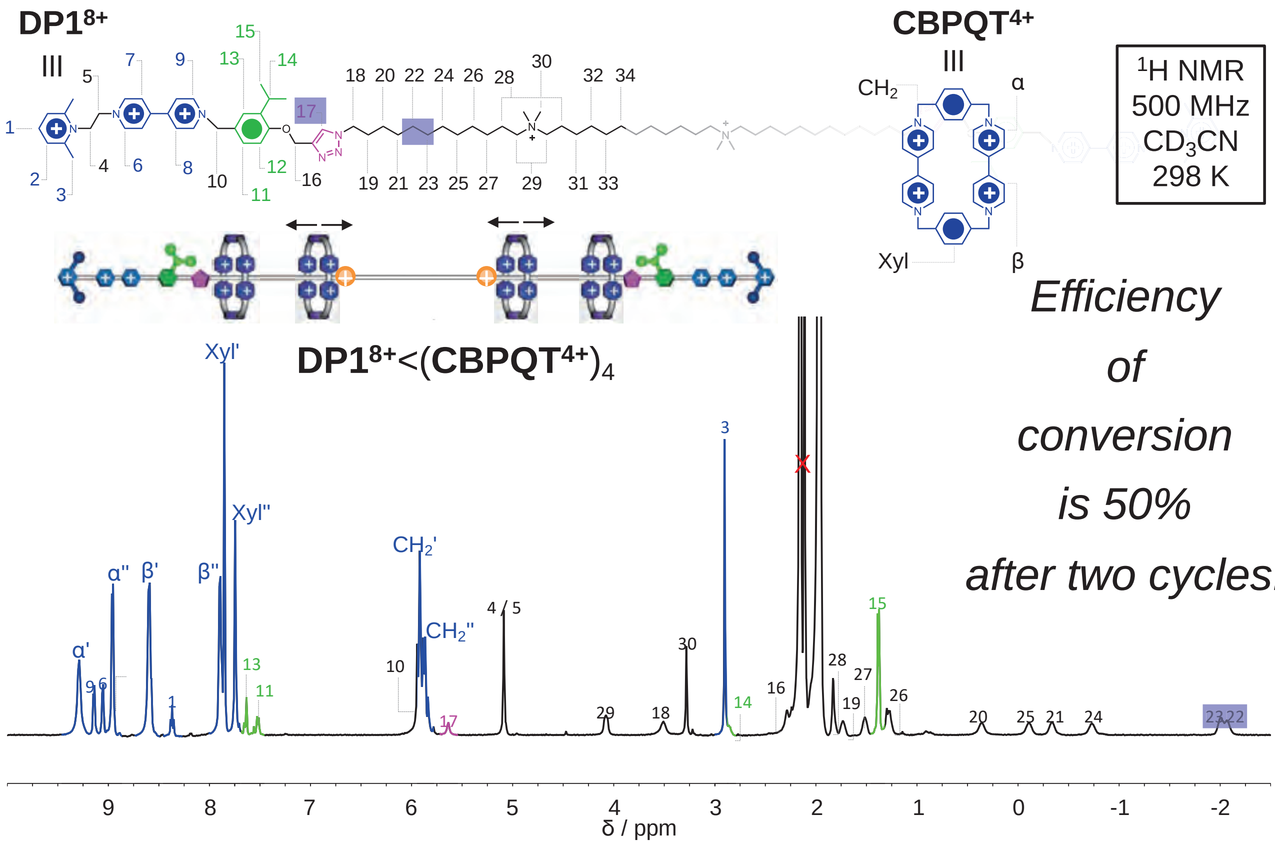
Angew. Chem. Int. Ed. **2018**, 57, 9325–9329

PUMP OPERATION AND COULOMETRY / 2



Angew. Chem. Int. Ed. **2018**, 57, 9325–9329

AFTER TWO CYCLES / [5]ROTAXANE



Efficiency of conversion is 50% after two cycles!

Angew. Chem. Int. Ed. **2018**, *57*, 9325–9329

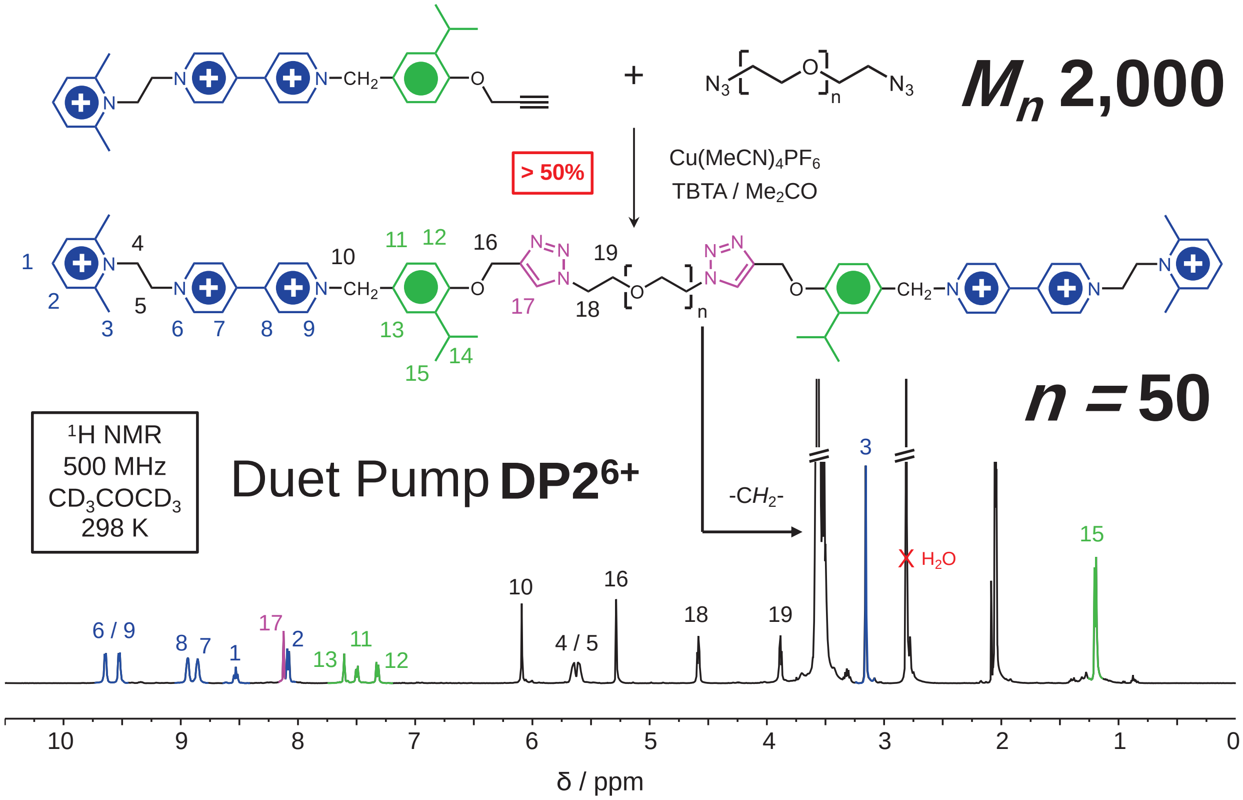
ACS FRONTIERS FRIDAY ROADMAP

Radical Chemistry | Feashing Energy Ratchets | Away-From-Equilibrium | Mechanisorption

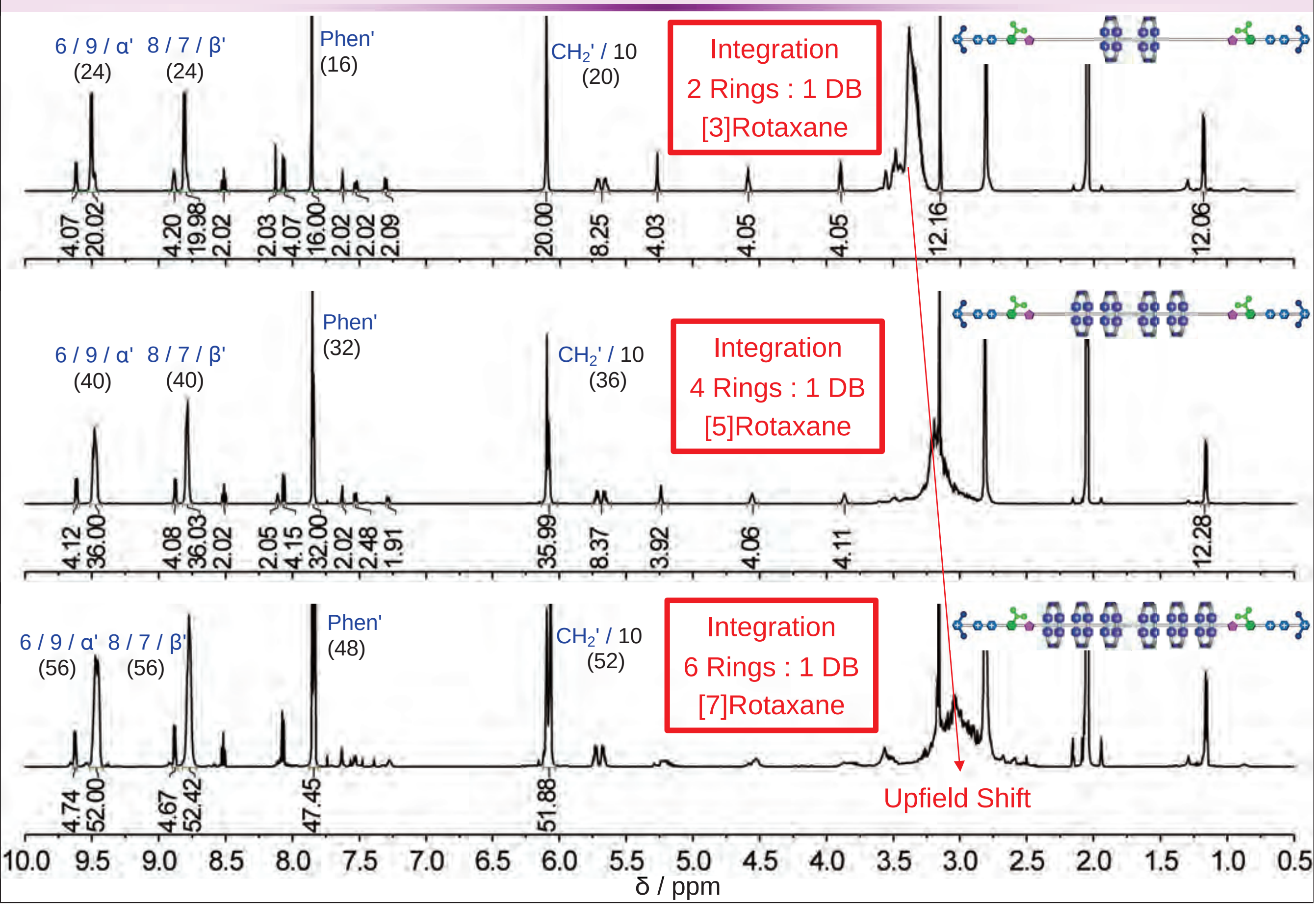
Molecular Pumps Mark I & II → **[3]Catenane Electric Motor** → **Molecular Dual & Duet Pumps** → **Precise Polyrotaxane Synthesizer**

TOWARD POLYCATIONIC POLYROTAXANES

Mark II Design *...a model polymeric duet pump...*



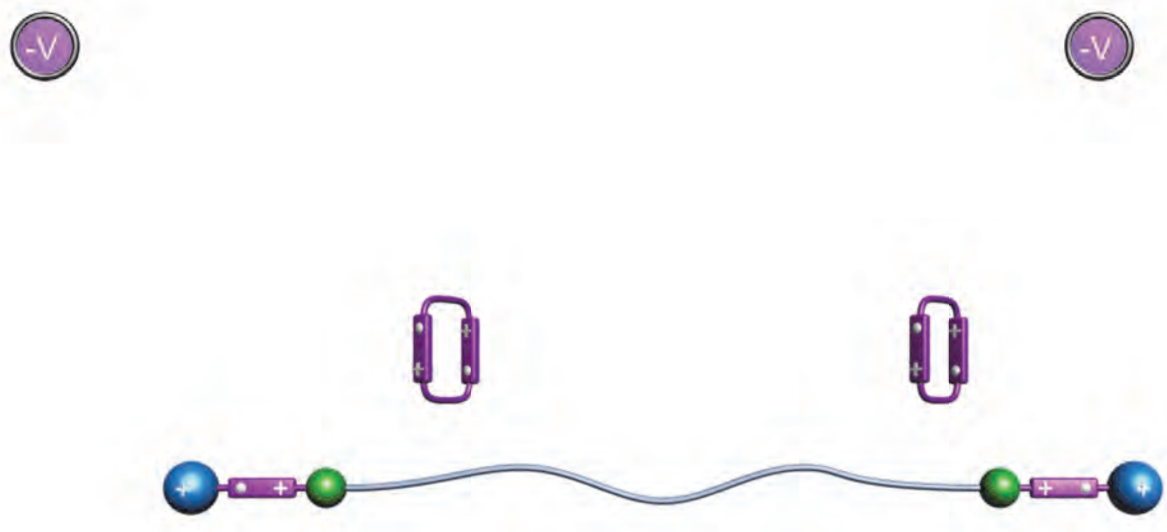
SEQUENTIAL CHEMICAL SYNTHESIS OF POLYROTAXANES



POLYROTAXANE SYNTHESIZER

Yunyan Qiu

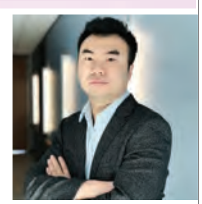
Yunyan Qiu



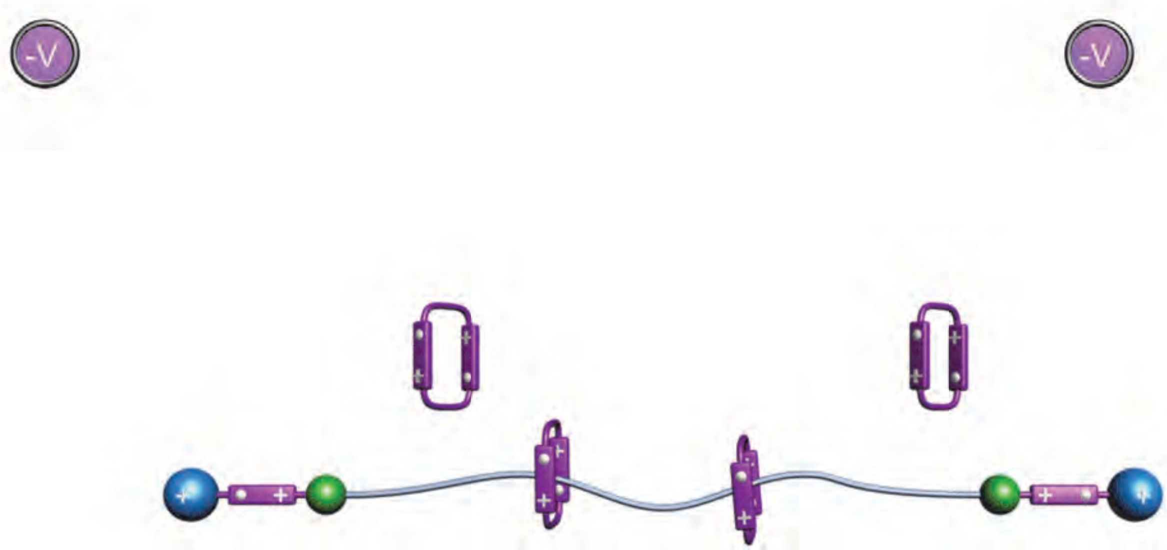
Science **2020**, *368*, 1247

POLYROTAXANE SYNTHESIZER

Yunyan Qiu



Yunyan Qiu



Science **2020**, *368*, 1247

POLYROTAXANE SYNTHESIZER

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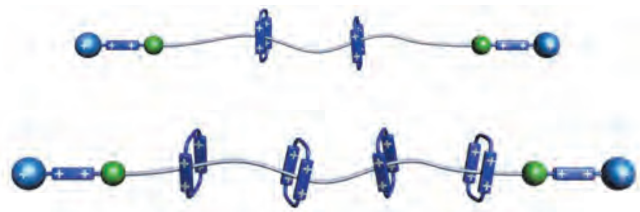
Yunyan Qiu



Science **2020**, *368*, 1247

POLYROTAXANE SYNTHESIZER

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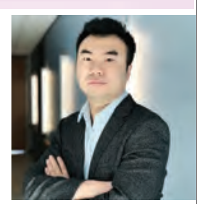
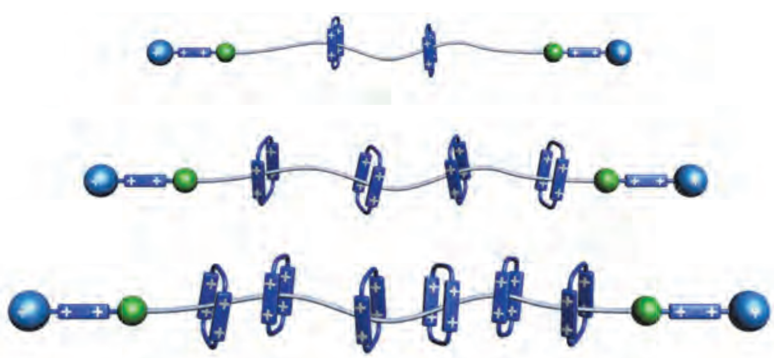
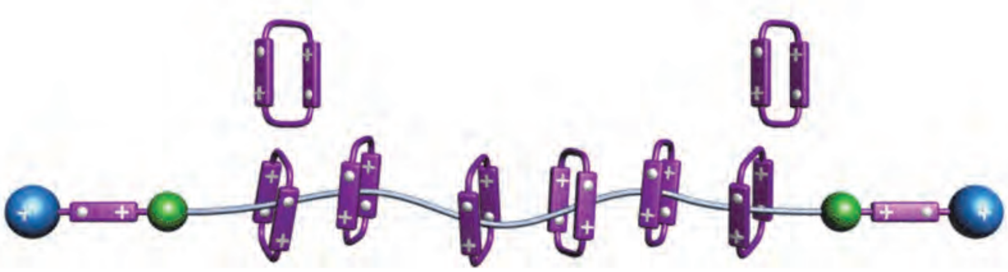


Yunyan Qiu



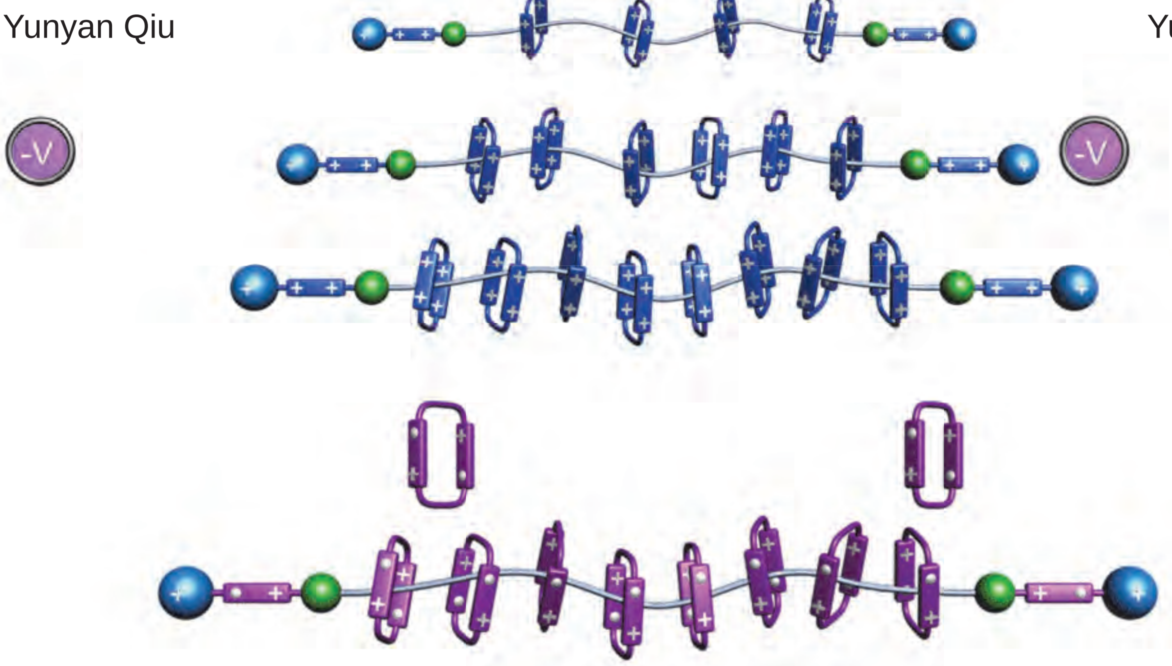


Science **2020**, *368*, 1247

POLYROTAXANE SYNTHESIZER

Yunyan Qiu

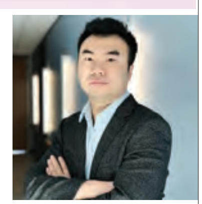
Yunyan Qiu



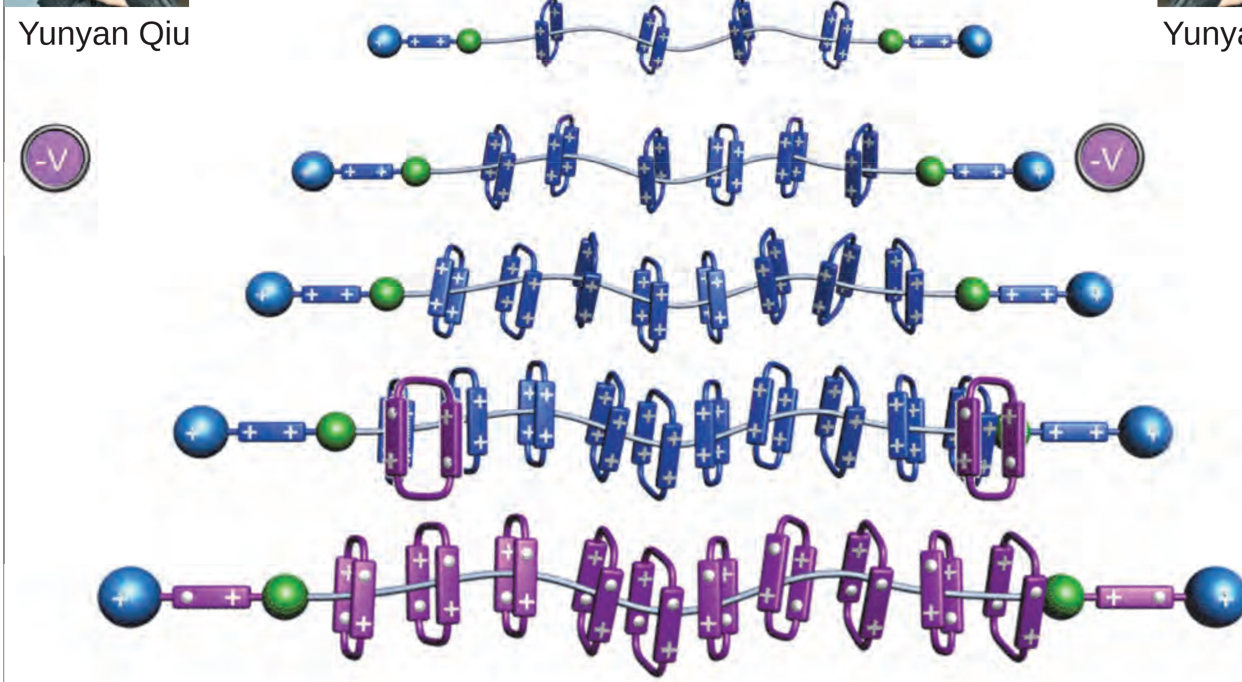
Science **2020**, *368*, 1247

POLYROTAXANE SYNTHESIZER

Yunyan Qiu



Yunyan Qiu



Science **2020**, *368*, 1247

WHAT MIGHT BE POSSIBLE?

Rings	2	4	6	8	10	12
+ve Charge	8	16	24	32	40	48

2 Stationary Charges — $\underbrace{\text{48 Movable Charges}}$ — 2 Stationary Charges

52 Overall

HAVE WE A NEW WAY TO MAKE

?ALL-ORGANIC BATTERIES?

PEG 5000 / TWO REDOX CYCLES

Repeating Controlled Potential Coulometry

PolyDB^{6+} / CBPQT^{4+}

1 eq : 10 eq

0.05 M $TBAPF_6$

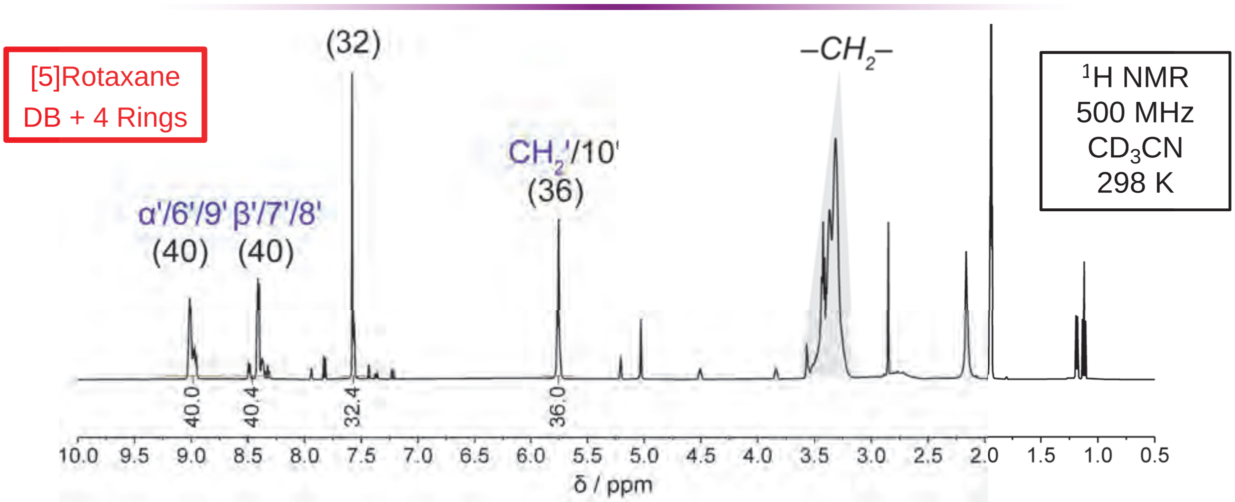
dry MeCN

Room Temp.

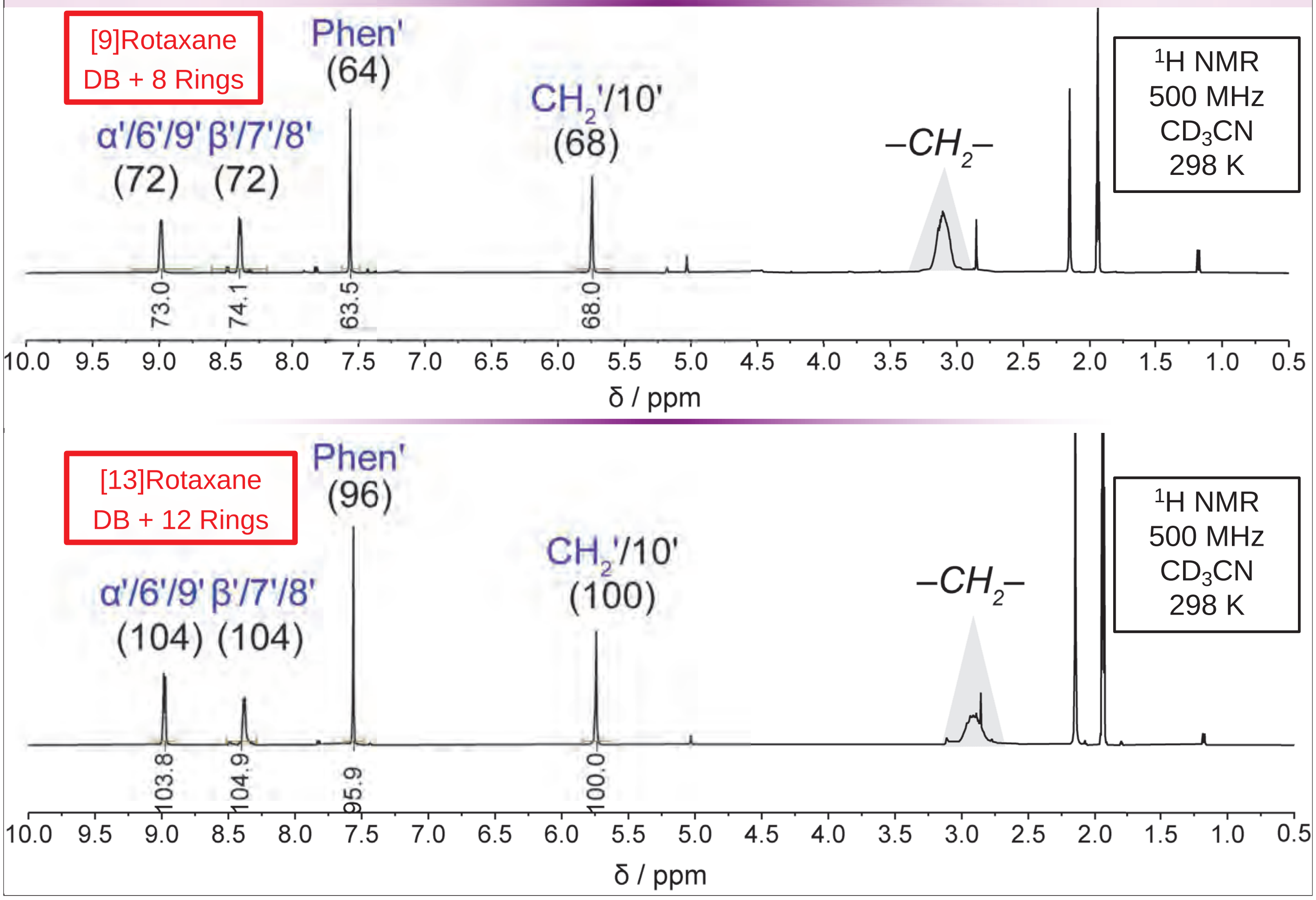
Reduction (-0.7 V)

Oxidation (+0.7 V)

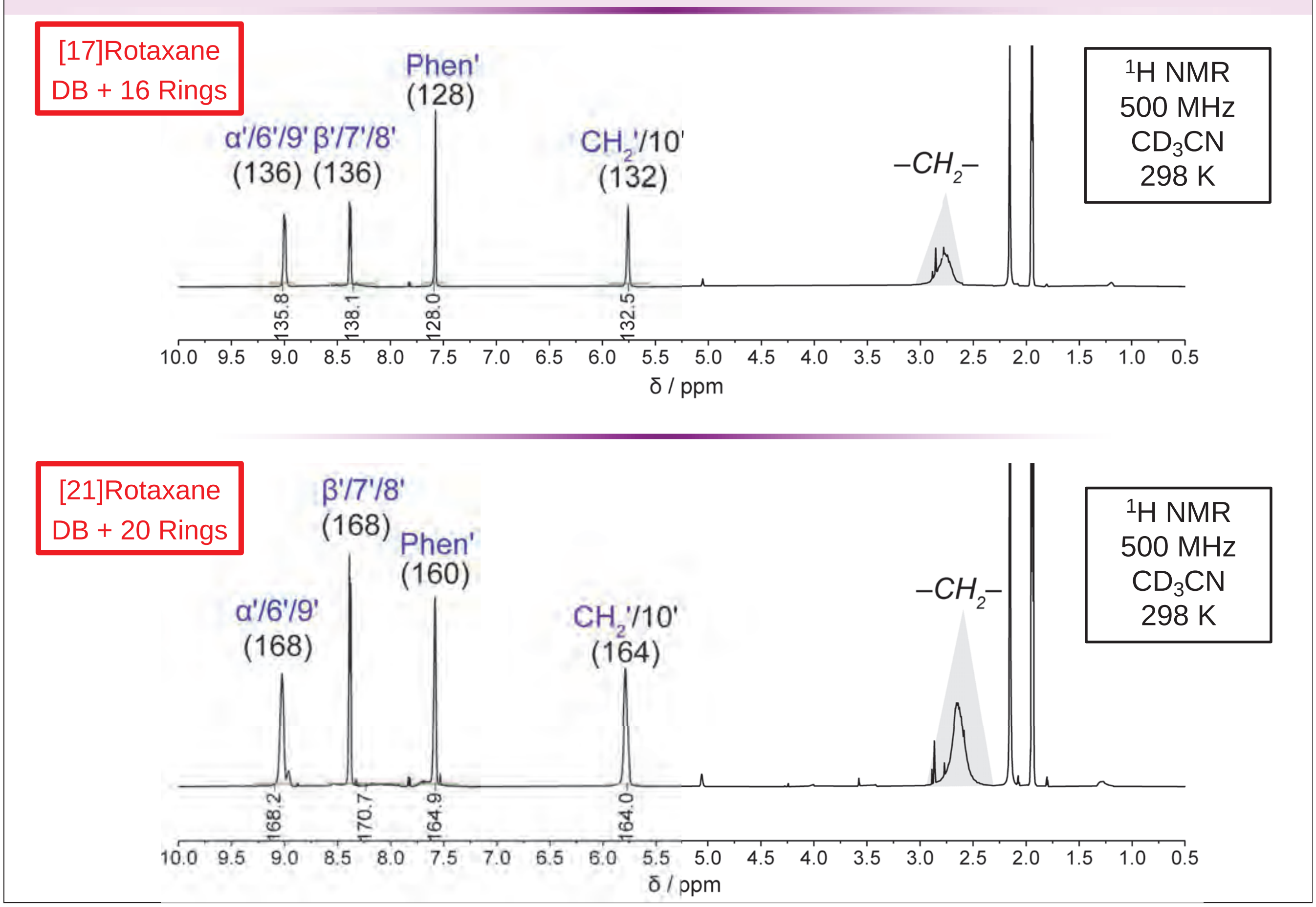
2 Redox Cycles



PEG 5000 / FOUR AND SIX REDOX CYCLES



PEG 5000 / EIGHT AND TEN REDOX CYCLES



EIGHT-ARM STAR PEG 20000 / SIX REDOX CYCLES

Repeating Controlled Potential Coulometry

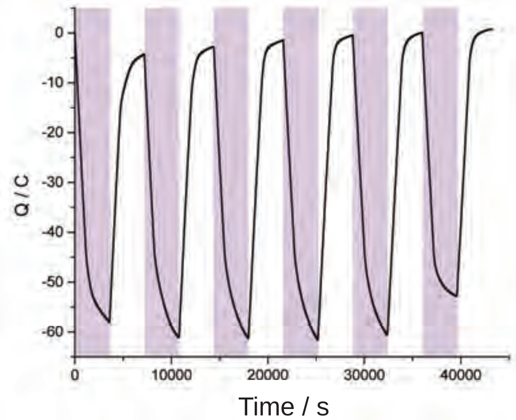
PolyDB^{24+} / CBPQT^{4+}

1 eq : 72 eq

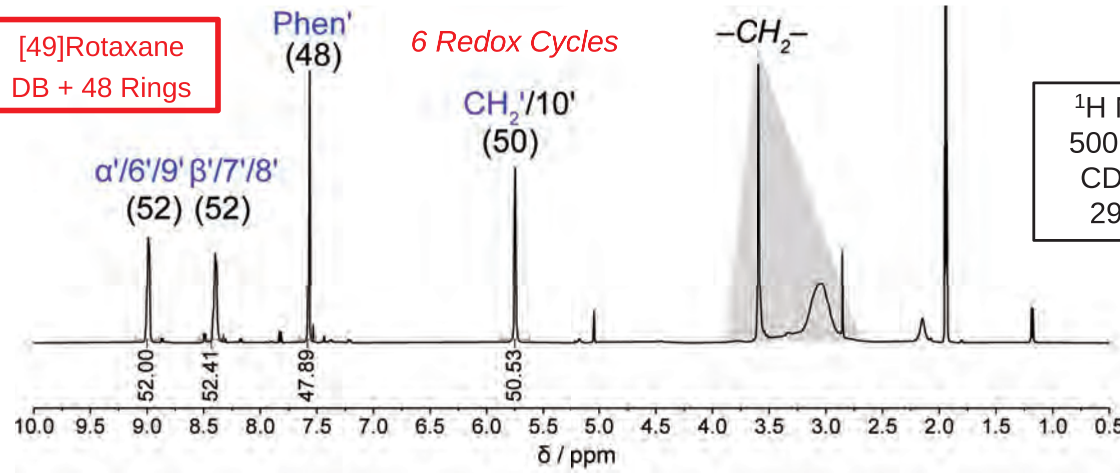
0.05 M $TBAPF_6$

dry MeCN

Room Temp.



[49]Rotaxane
DB + 48 Rings



^{1}H NMR
500 MHz
CD_3CN
298 K

TAKE HOME MESSAGES SO FAR

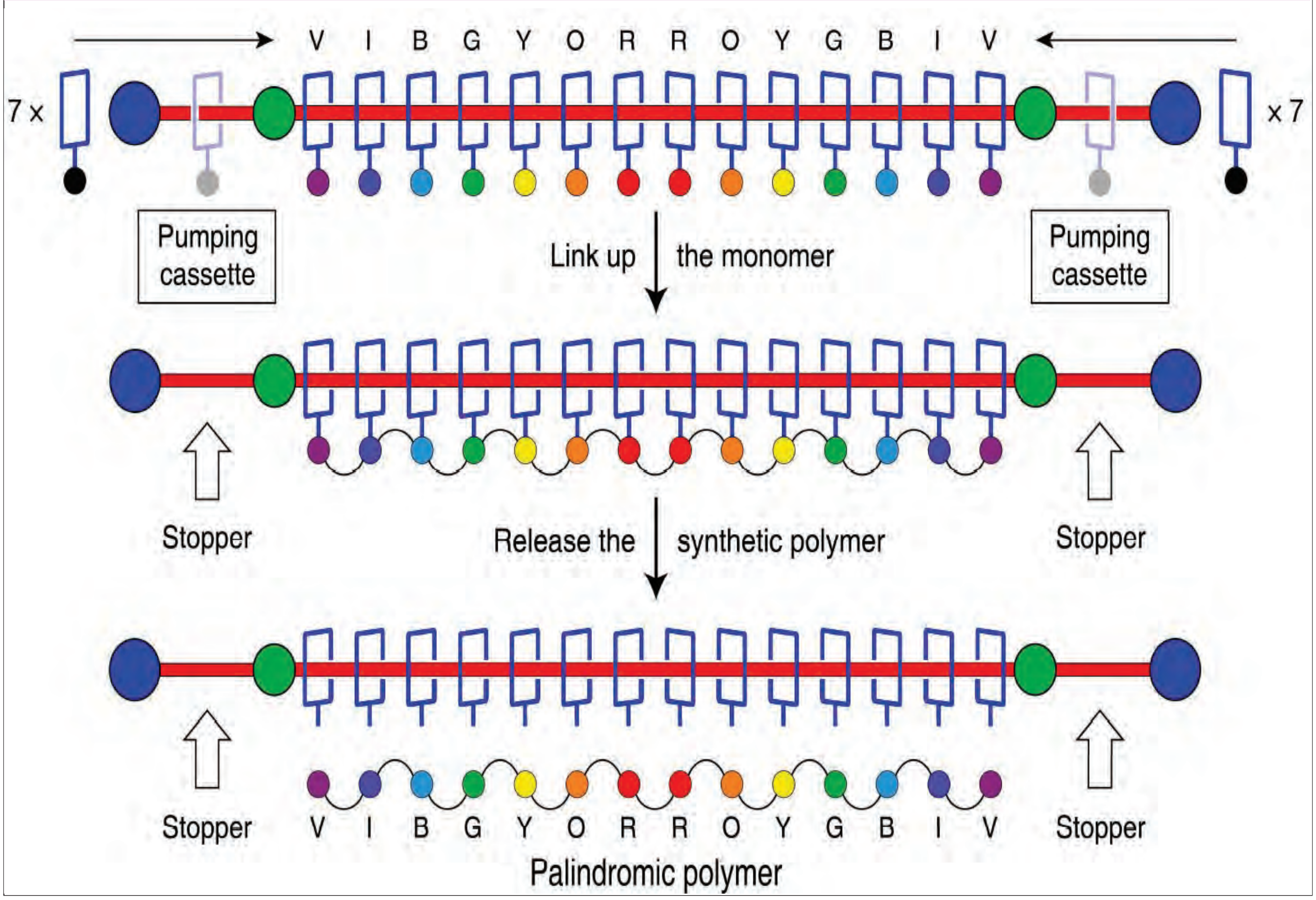
The controlled synthesis of polyrotaxanes
through an autonomous electrochemical approach
using artificial molecular pumps

The installment of up to 20 rings onto a linear PEG polymer
(MW 5000) with a total of
86 positive charges!!!

The installment of up to 80 rings onto a star PEG polymer
(MW 20000) with a total of
344 positive charges!!!

HAVE WE A NEW WAY TO MAKE
ALL-ORGANIC BATTERIES?

MECHANICAL BONDING-INDUCED SITE-SELECTIVE FUNCTIONALIZATION



ACS FRONTIERS FRIDAY ROADMAP

Radical Chemistry | Flashing Energy Ratchets | Away-From-Equilibrium | Mechanisorption

Molecular Pumps Mark I & II → **[3]Catenane Electric Motor** → **Molecular Dual & Duet Pumps** → **Precise Polyrotaxane Synthesizer** → **Robust Dynamics MIMs on MOFs** → **Physisorption Chemisorption Mechanisorption**

Outlook for Molecular Nanotechnology

OUTLOOK FOR MOLECULAR NANOTECHNOLOGY BASED ON CHEMICAL FUELS AND ELECTRICITY

Kinetics control AMMs | AMPs

- Kinetics provide the foundation for developing AMMs | AMPs.
- Kinetics are important in creating and maintaining non-equilibrium states.
- Kinetics have led to the development of pumping cassettes in AMPs.

Radicals provide the Driving Force

- Radical-pairing is a powerful way of driving molecular assembly and motion.
- Radical-pairing provides us with powerful forces to module energy barriers.
- Radical-pairing has led to the design and use of pumping cassettes.

Pumping Cassettes create Far-From-Equilibrium System

- Externally driven AMMs | AMPs operatre by using energy ratchets.
- Energy ratchets produce away-from-equilibrium AMMs | AMPs.
- AMPs when attached to surfaces can produce non-equilibrium systems.

Mechanisorption

AMMs ≡ Artificial Molecular Machines

AMPs ≡ Artificial Molecular Pumps

THE RADICAL CHEMISTS

Radical-Pairing-Induced Molecular Assembly and Motion
Nat. Rev. Chem. In Press

A Radical Departure For Supramolecular Chemistry
Nat. Rev. Chem. In Press

THE RADICAL SCIENTISTS

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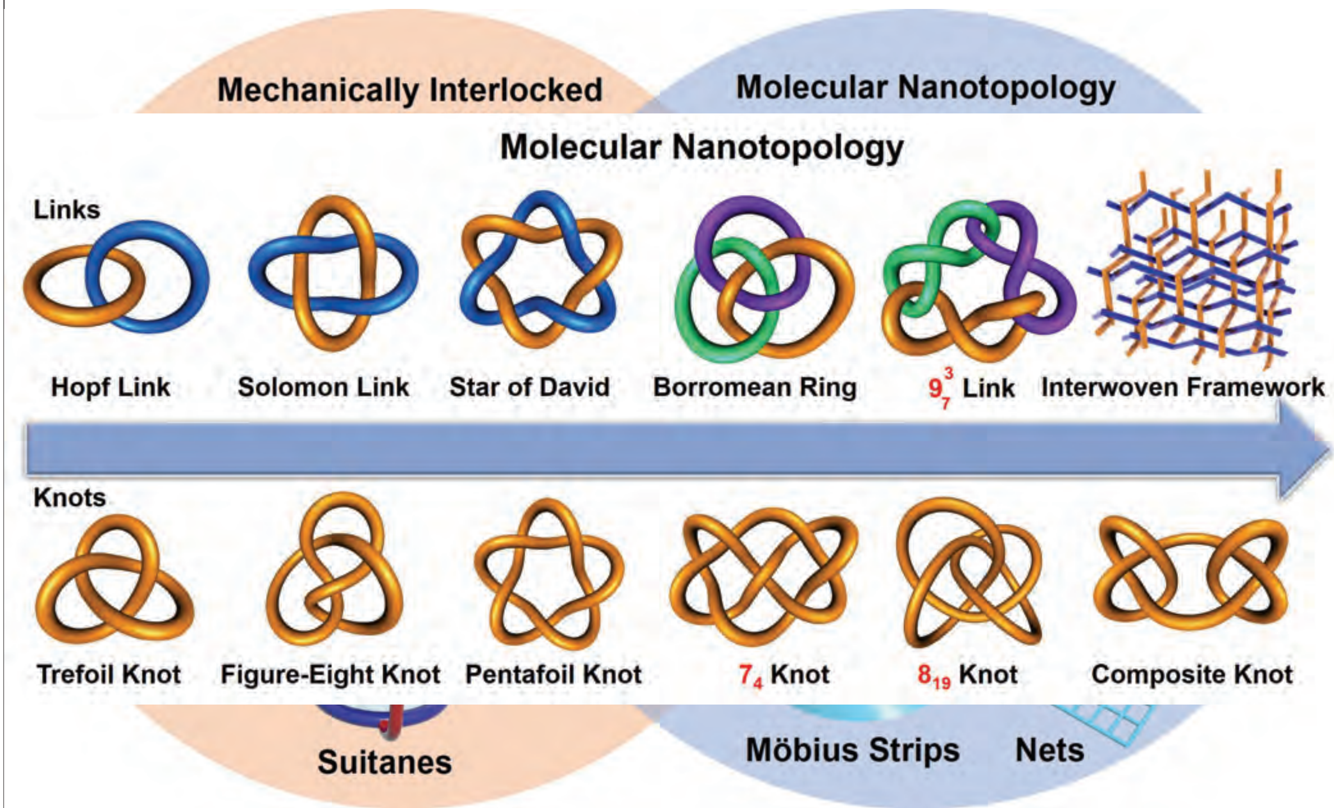
Outlook for Molecular Nanotechnology

The Rise and Promise of Molecular Nanotopology

Nano Lett. **2020**, *20*, 5597–5600 | *CCS Chem.* **2021**, *3*, 1542–1572

THE RISE AND PROMISE OF MOLECULAR NANOTOPOLOGY



Nano Lett. **2020**, *20*, 5597–5600 | *CCS Chem.* **2021**, *3*, 1542–1572

CROP OF LOCKDOWN REVIEWS

Pumps through the Ages	*Chem* **2020**, *6*, 1952–1977
Dawning of the Age of Molecular Nanotopology	*Nano Lett*. **2020**, *20*, 5597–5600
Cyclodextrin Metal-Organic Frameworks and Their Applications	*Acc. Chem. Res*. **2021**, *54*, 1440–1453
Emergent Behavior in Nanoconfined Molecular Containers	*Chem* **2021**, *7*, 919–947
Molecular Triangles: A New Class of Macrocycles	*Acc. Chem. Res*. **2021**, *54*, 2027–2039
Molecular Pumps and Motors	*J. Am. Chem. Soc.* **2021**, *143,* 5569–5591
Aromatic Hydrocarbon Belts	*Nat. Chem.* **2021**, *13,* 402–419
The Rise and Promise of Molecular Nanotopology	*CCS Chem.* **2021**, *3*, 1542–1572
Radical-Pairing-Induced Molecular Assembly and Motion	*Nat. Rev. Chem.* **2021**, *5*, In Press
From Molecular to Supramolecular Electronics	*Nat. Rev. Mater.* **2021**, *6*, In Press

Coming Soon

Chiroptical Properties of Mechanically Interlocked Molecules	*Israel J. Chem.*
Whither Second-Sphere Coordination?	*CCS Chem.*

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Artificial Molecular Machines

Going from Solution to Surfaces

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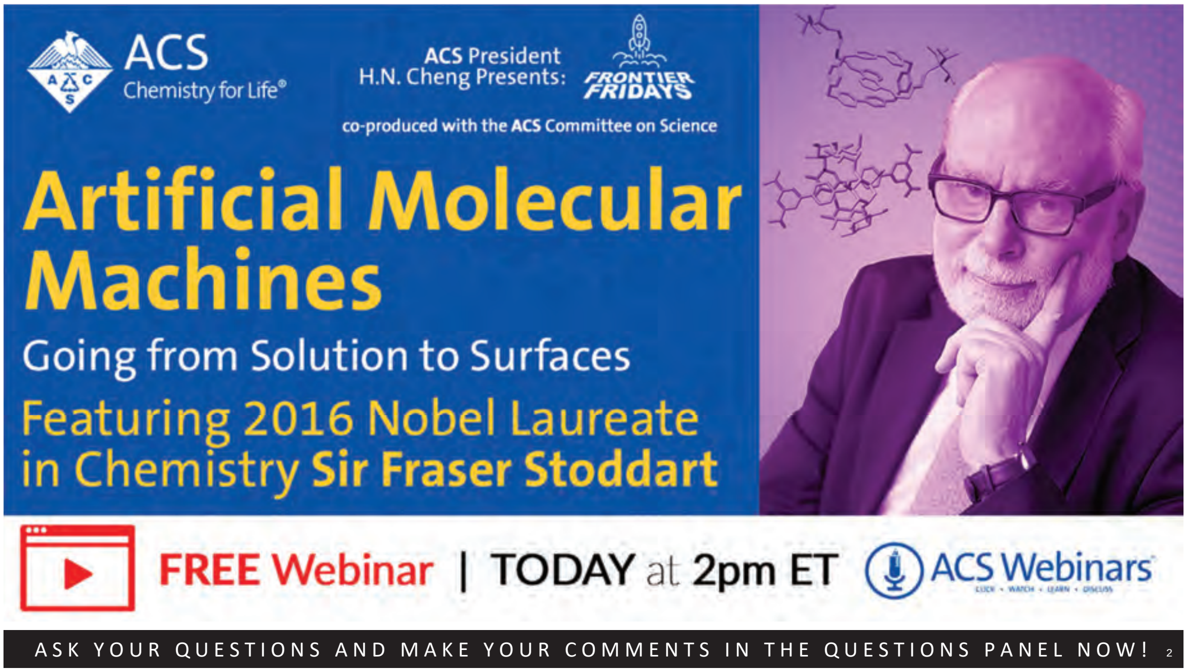

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Chemistry for Life®

Chemistry on Capitol Hill
2021 Emerging Policies

Date: Wednesday, June 30, 2021 @ 2-3pm ET
Speakers: Caroline Trupp Gil, American Chemical Society / Karen Garcia, American Chemical Society / Carl Maxwell, American Chemical Society
Moderator: Lauren Posey, American Chemical Society

Register for Free!

What You Will Learn:

- How the Biden Administration and 117th Congress are shaping up in terms of its STEM priorities
- Which specific pieces of legislation or federal policies will be likely to impact ACS members
- How members can become involved

Co-produced with: ACS Government Affairs

Designing Bio-Sourced Polymers
that Enable Recycling

Date: Thursday, July 1, 2021 @ 2-3pm ET
Speaker: Stefan Mecking, University of Konstanz
Moderator: Mark Jones, Dow Chemical (retired)

Register for Free!

What You Will Learn:

- What is solvolysis and how it can enable plastics recycling
- How renewable polycarbonates and polyesters with a low density of in-chain functional groups as break points in a polyethylene chain can be recycled chemically
- How long-chain building blocks for polycondensation can be created from common plant oil feedstocks or microalgae oils

Co-produced with: ACS Division of Polymer Chemistry

Succeeding in a Global Environment
Successfully Working Across Cultures

Date: Wednesday, July 7, 2021 @ 2-3pm ET
Speaker: Ramki Subramnian, DowAksa USA
Moderator: Tom Halleran, American Chemical Society

Register for Free!

What You Will Learn:

- Why there are many aspects to culture and what are some of the many similarities & differences across those aspects
- Why your ability to work effectively across cultures is an important contributor to success
- How your overall career is a marathon, but the environment can change rapidly, requiring you to constantly observe and adapt to the culture around you

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