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From novel therapies, AI, materials, energy, & more…

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Introductions

Dr. Jonathan Allen

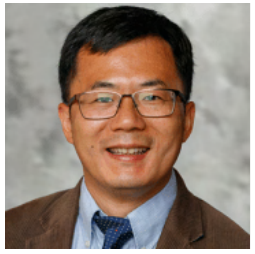
Informaticist team lead for small molecule drug discovery with AI/ ML at

Lawrence Livermore National Laboratory

Dr. Arnold Lumsdaine

Director of Innovation (INFUSE)

Oak Ridge National Lab



Dr. Yiying Wu

Professor of Chemistry specializing in energy storage and batteries

The Ohio State University

Janet Sasso

Information Scientist specializing in life sciences and biotechnology

CAS

Dr. Kevin Hughes

Information scientist specializing in materials science and applied physics

CAS

Dr. Angela Zhou

Manager scientific insight and analysis

Moderator

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TACKLING THE UNDRUGGABLES

Advancements and Emerging Trends

Janet Sasso, Information Scientist, CAS

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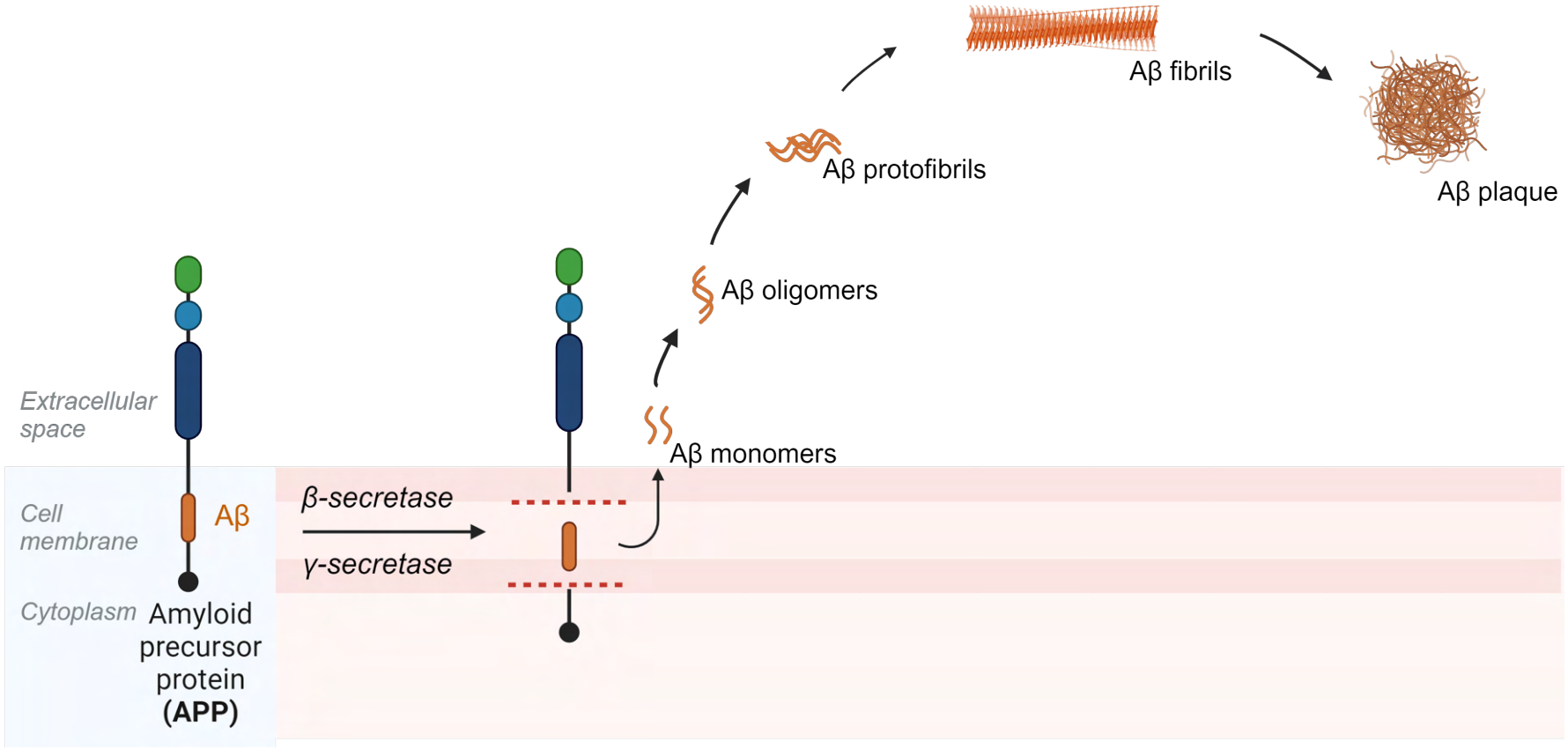
Alzheimer’s disease and emerging trends

Anti-amyloid agents



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Alzheimer’s disease and emerging trends

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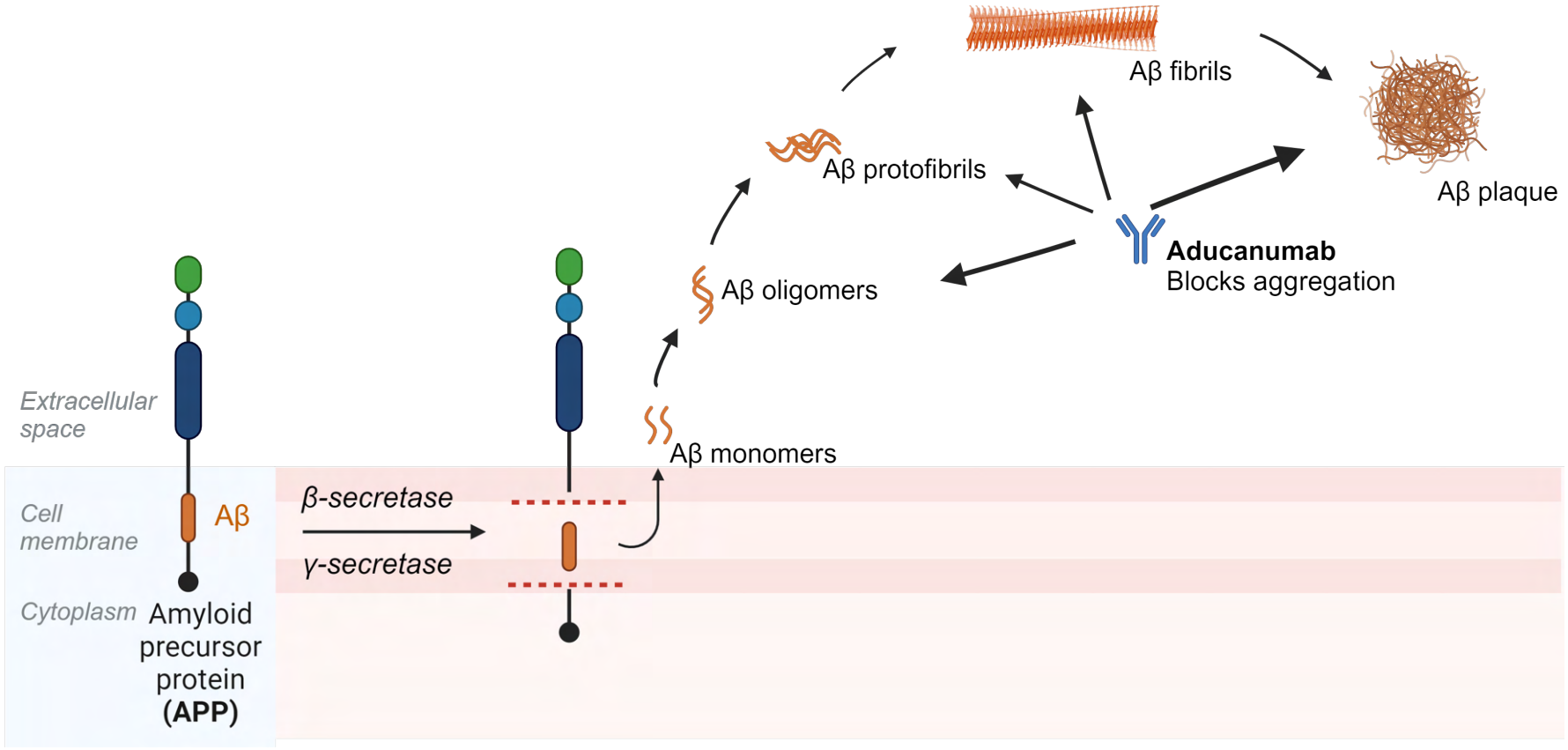

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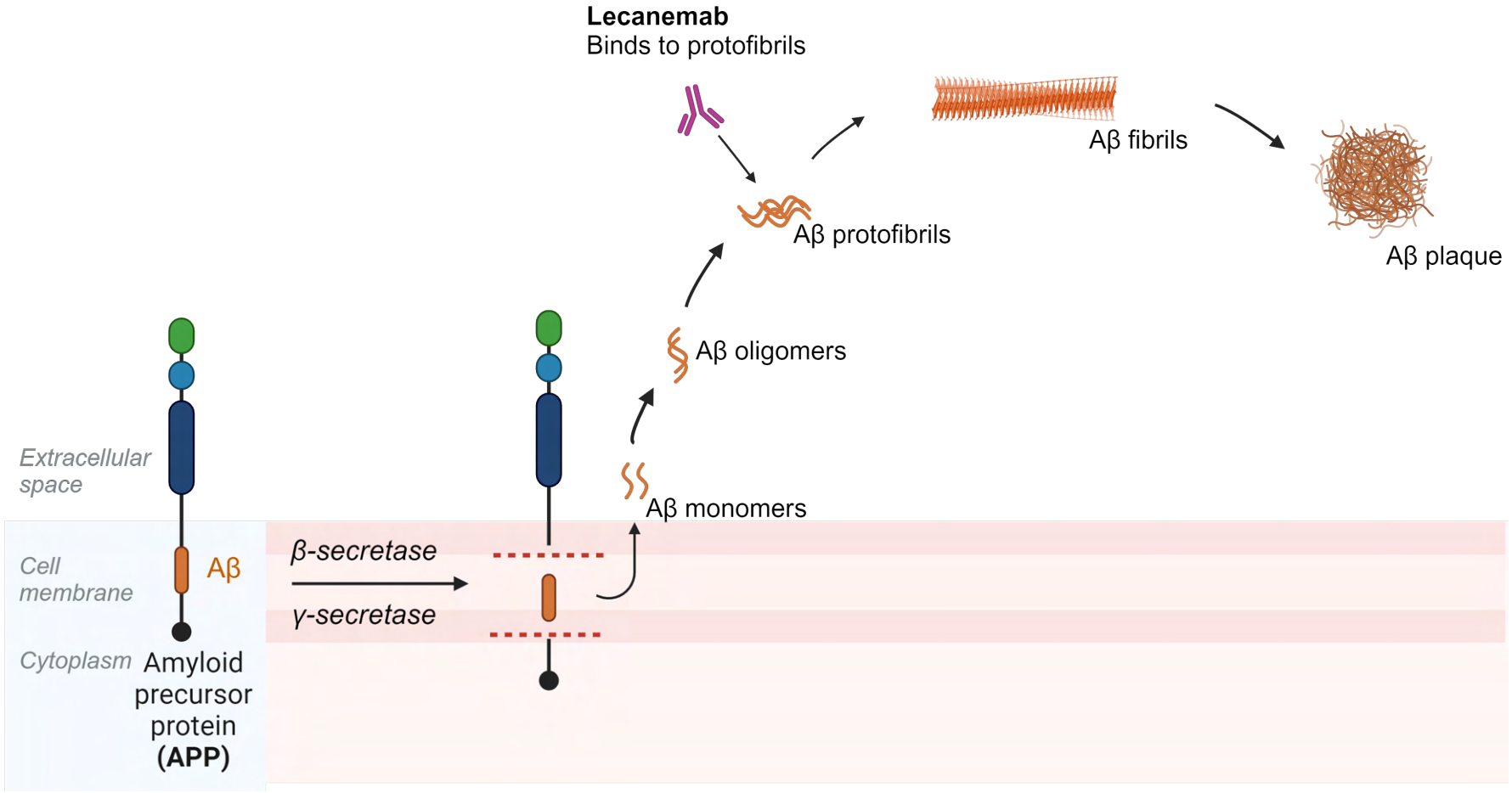

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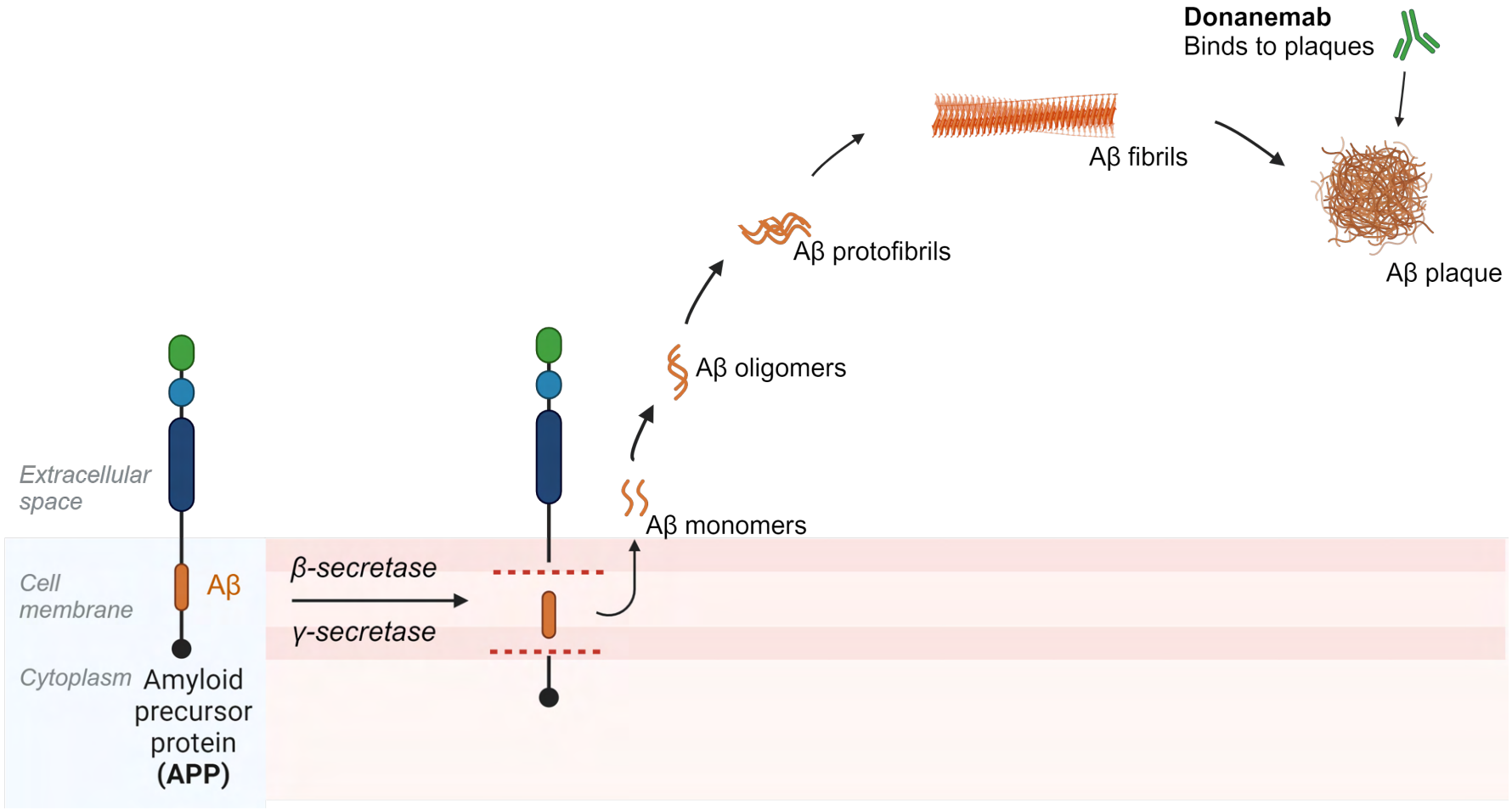

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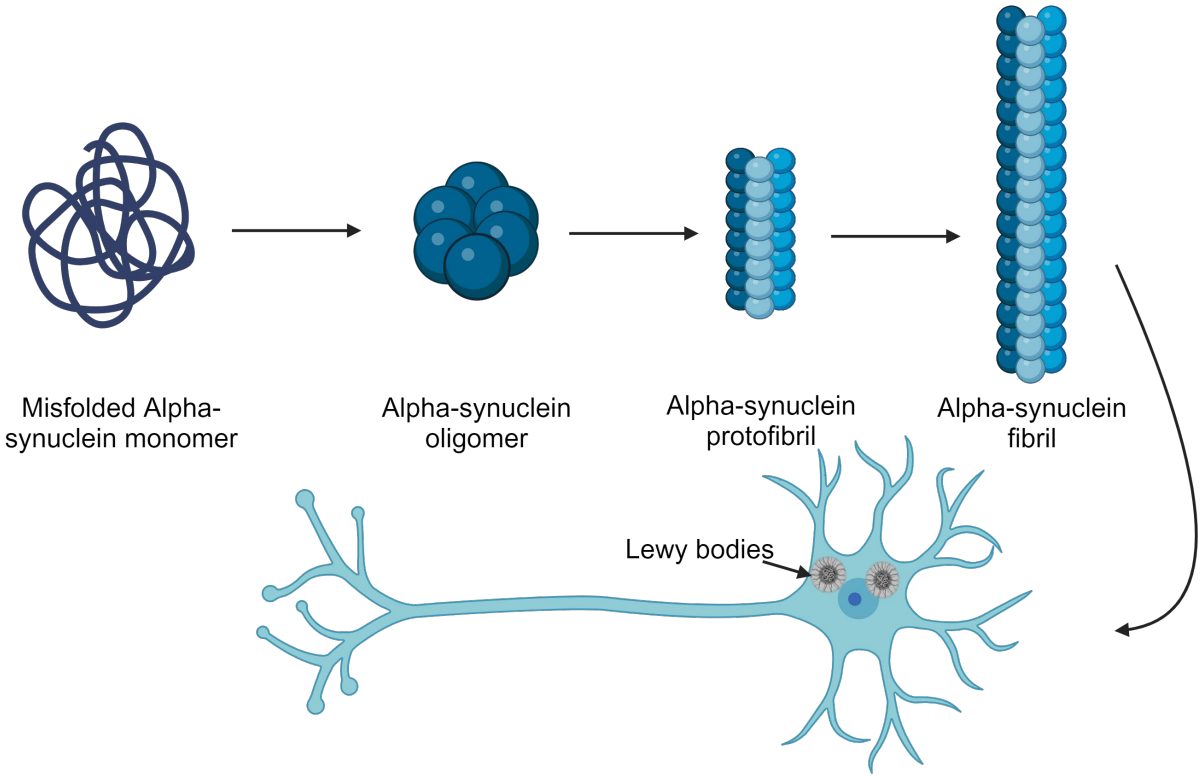
Parkinson’s disease and biomarker validation

Alpha-Synuclein



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Parkinson’s disease and biomarker validation

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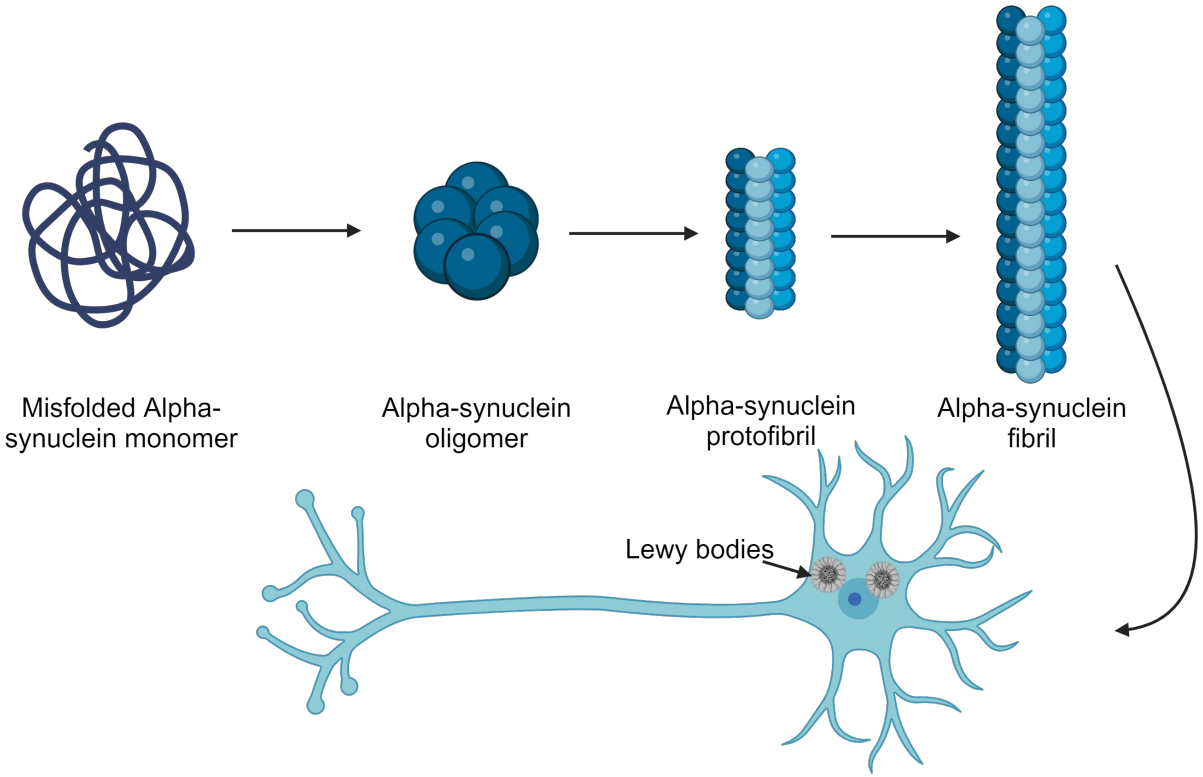

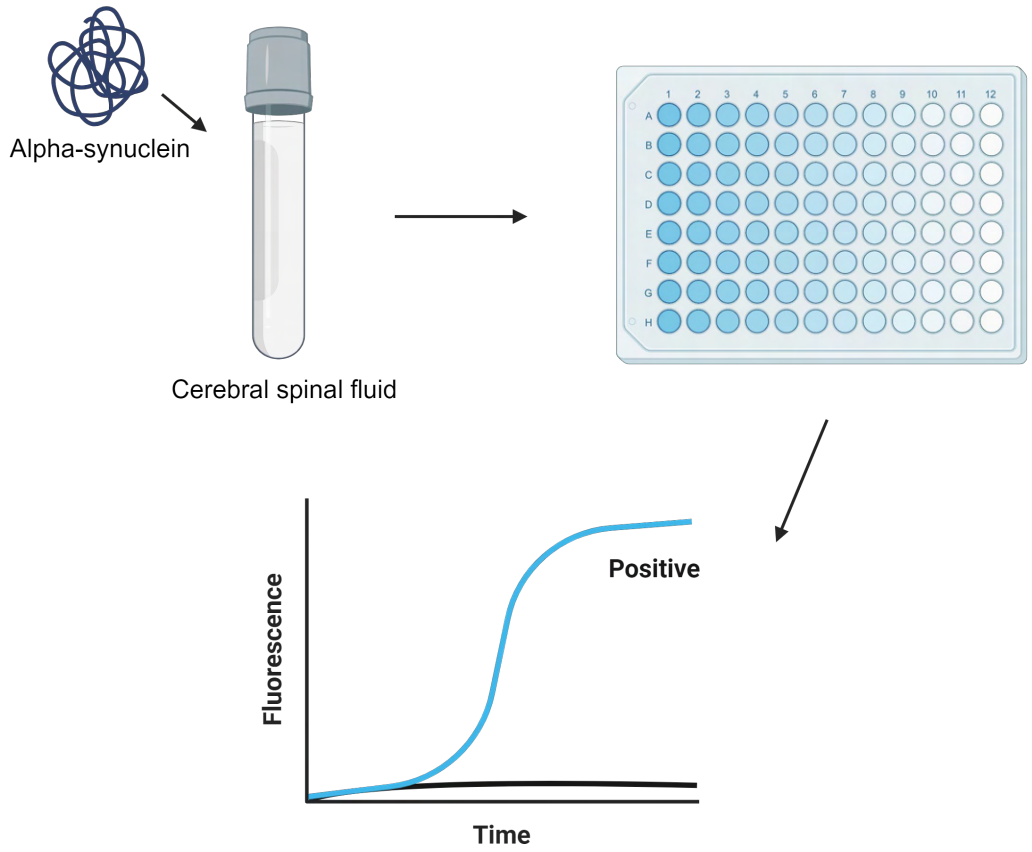

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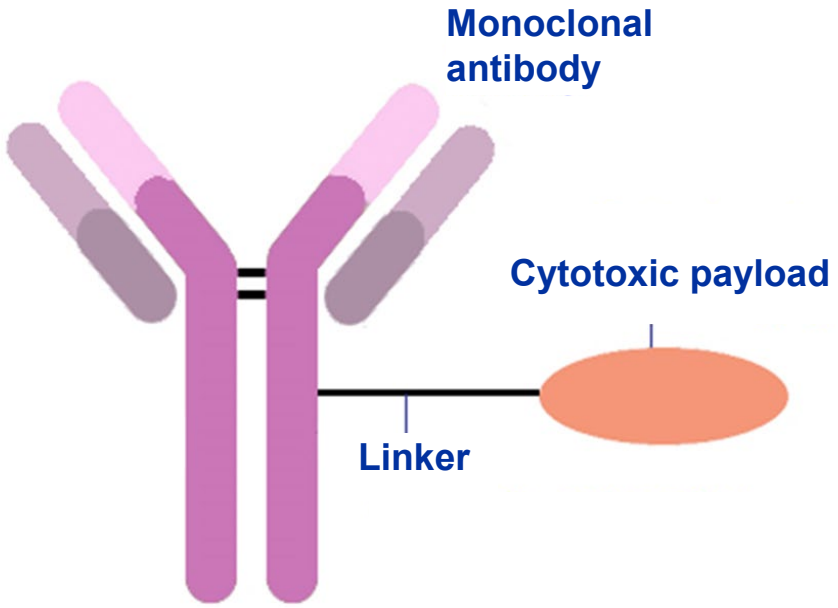
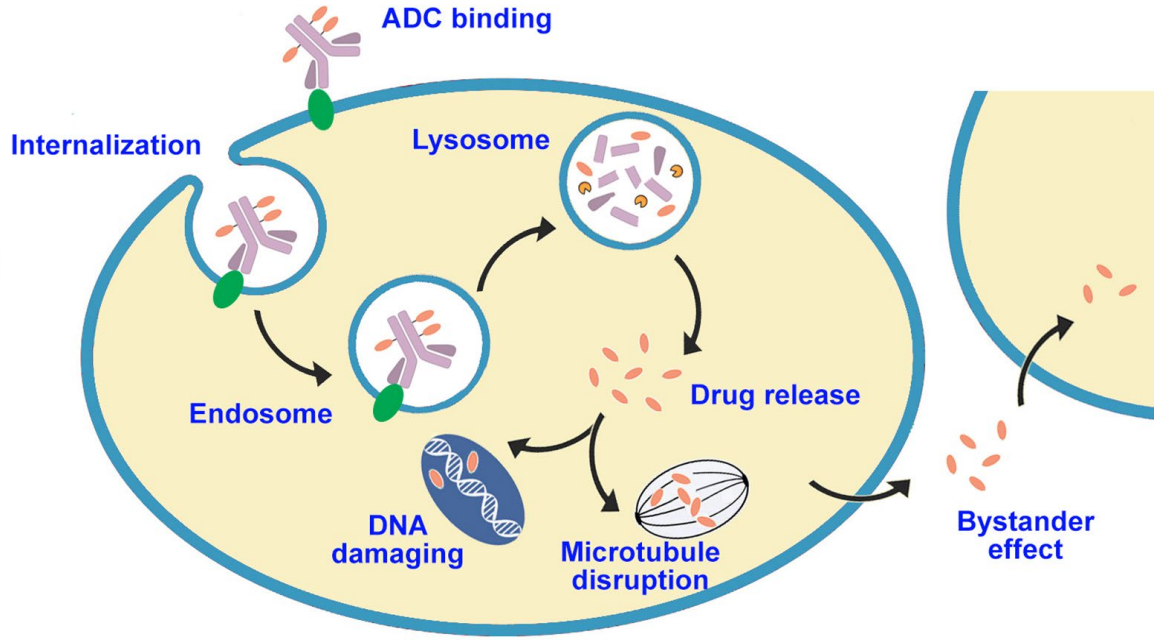
Antibody-drug conjugate (ADC)

Targeted Immunotherapeutic





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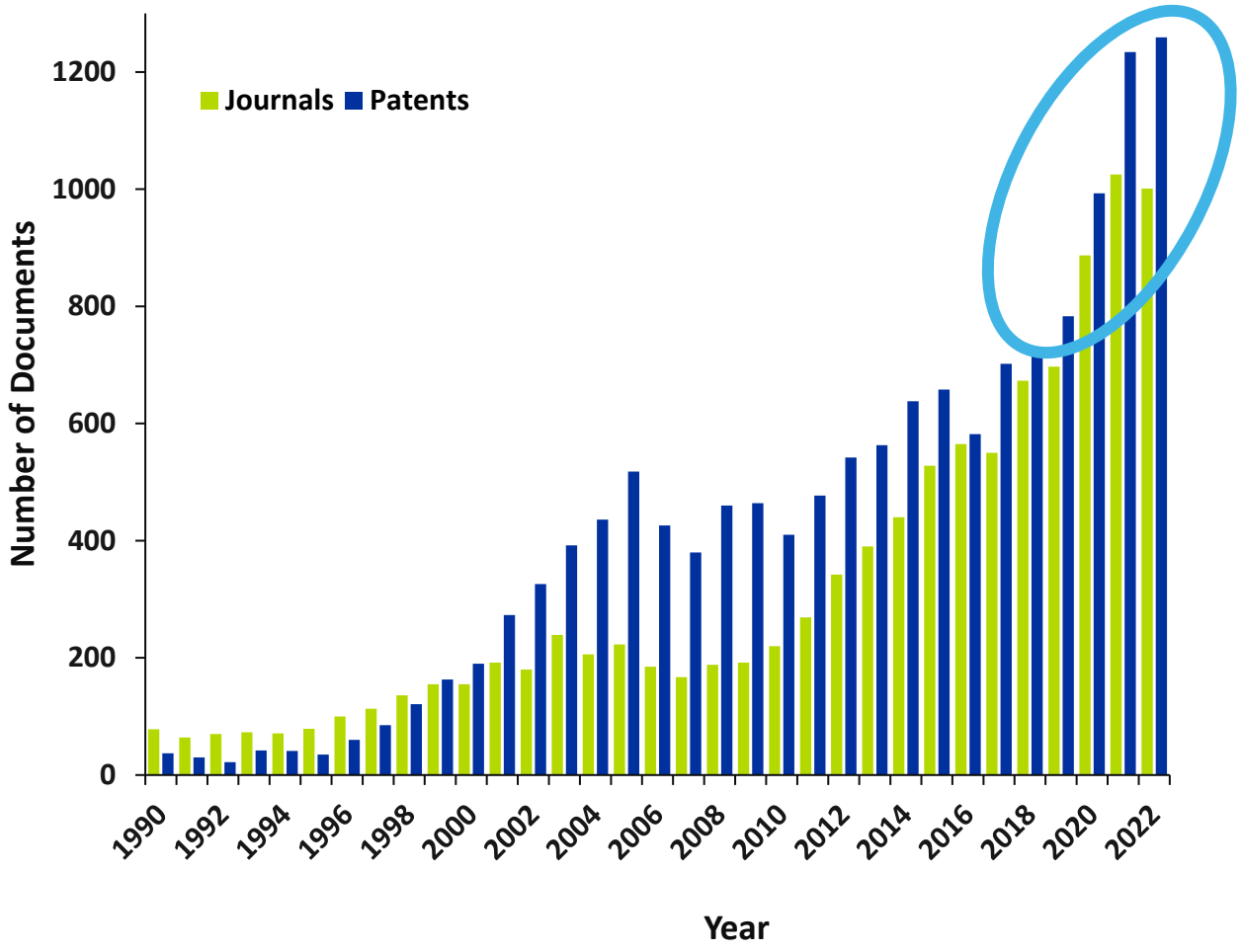
ADC Publication Trends

50x increase in patent publications since 1990s



Global patent trend for ADCs from 1990 to 2022 (CAS Content Collection™)

Trends

- Despite a pandemic, explosive growth of publications since first FDA approved ADC in 2000
- Nearly 30% increase in patents alone from 2020 onward

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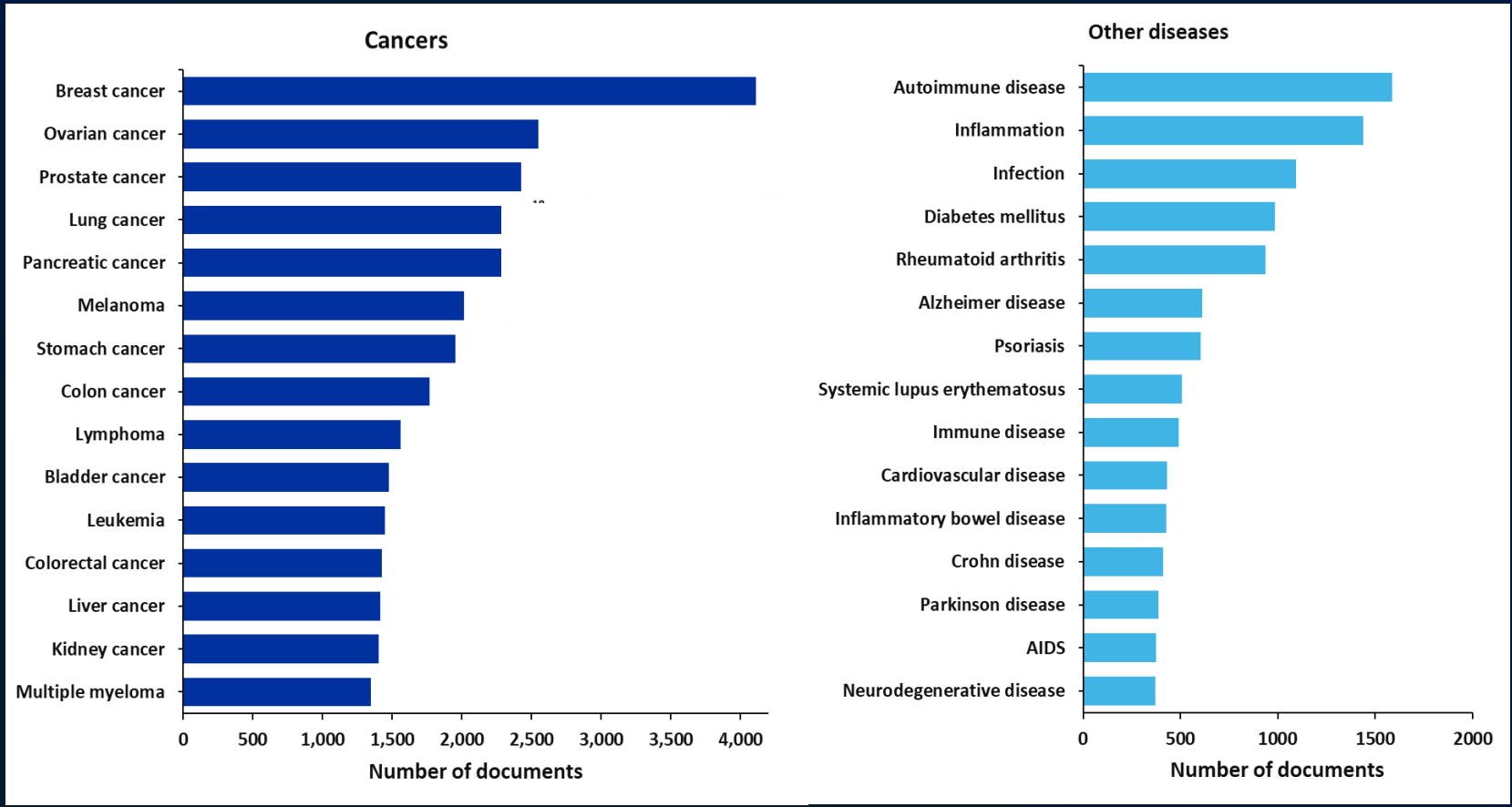
Oncology is leading the clinical pipeline

Expanding efforts to fill gaps left by conventional drugs



Trends

- Breast cancer and autoimmune disease lead paper publications
- Latest FDA ADC approvals target ovarian, head and neck, cervical, and gastric cancers.
- Outside of oncology, ADCs in clinical trials are exploring the treatment of autoimmune disorders and amyloidosis

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Janet Sasso
Information Scientist
jsasso@cas.org

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AI/ML developments in drug discovery

Jonathan Allen, Ph.D.
Informatics Scientist
allen99@llnl.gov

January 25, 2024

LLNL-PRES-859442

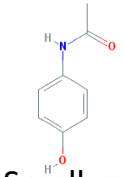
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Lawrence Livermore National Laboratory

Adding AI/ML decision making to drug discovery

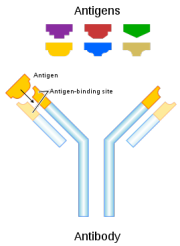
Traditional computational drug discovery approach

Drug types

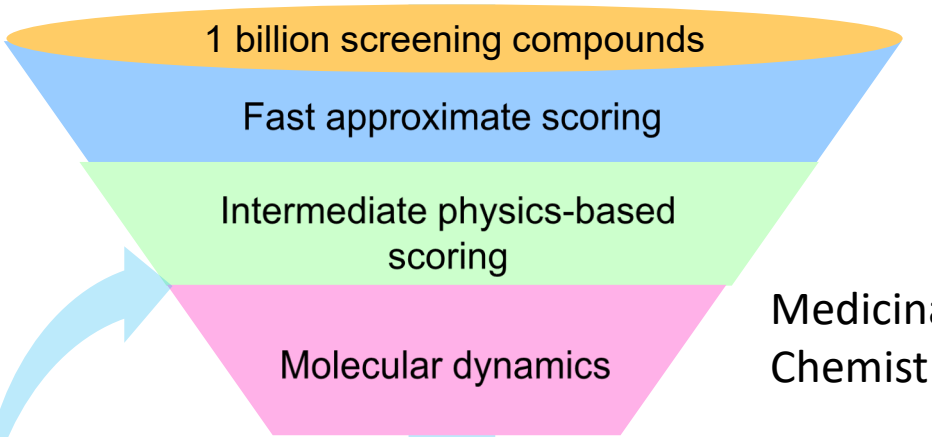


Small molecule

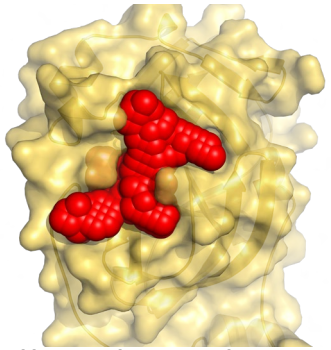
Peptide



Antibody
Antigen



Experimental feedback



Manually selected protein target

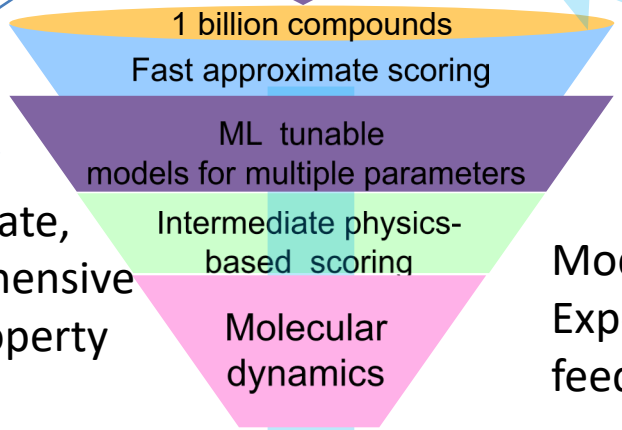
Medicinal Chemist

3) Intelligent search of chemical space

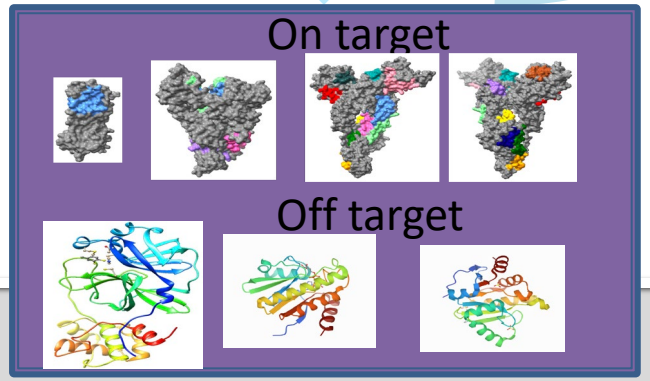
2) Accurate, comprehensive drug property scoring

1) Flexible on/off target selection for potency models

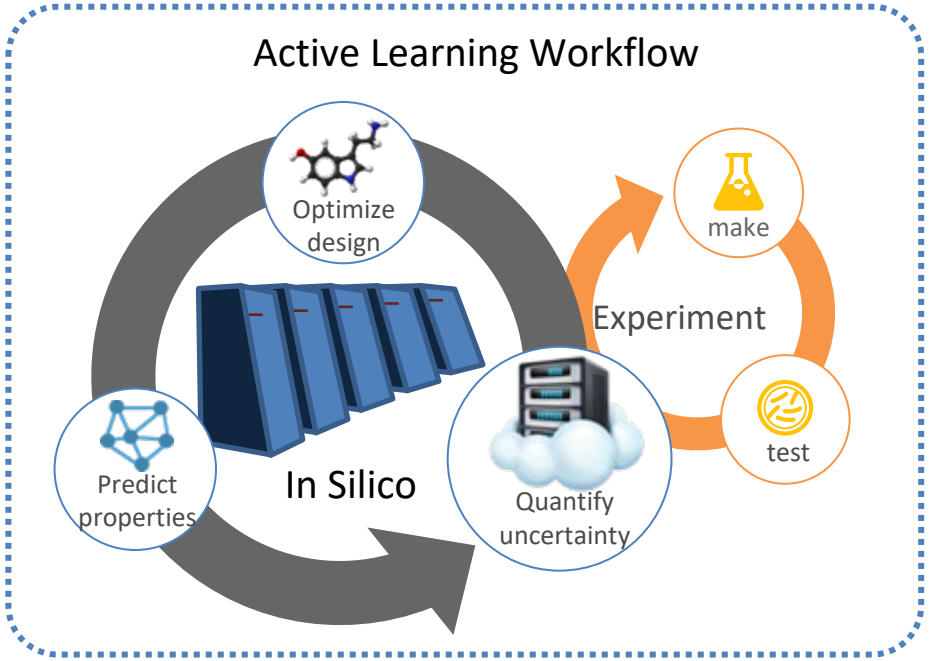
100+ billion screening compounds **Paradigm shift**



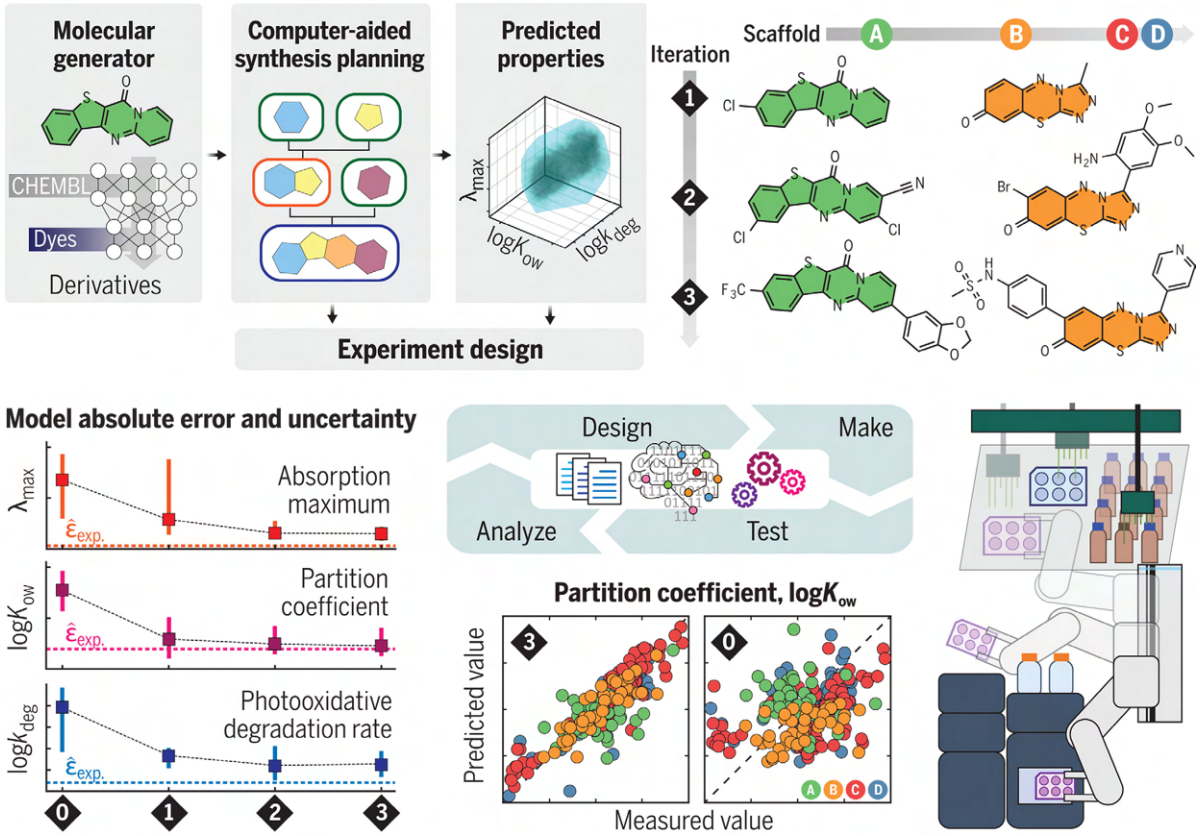
Model Driven Experimental feedback



Improved active learning workflows



Recent example of automated iterative chemical synthesis

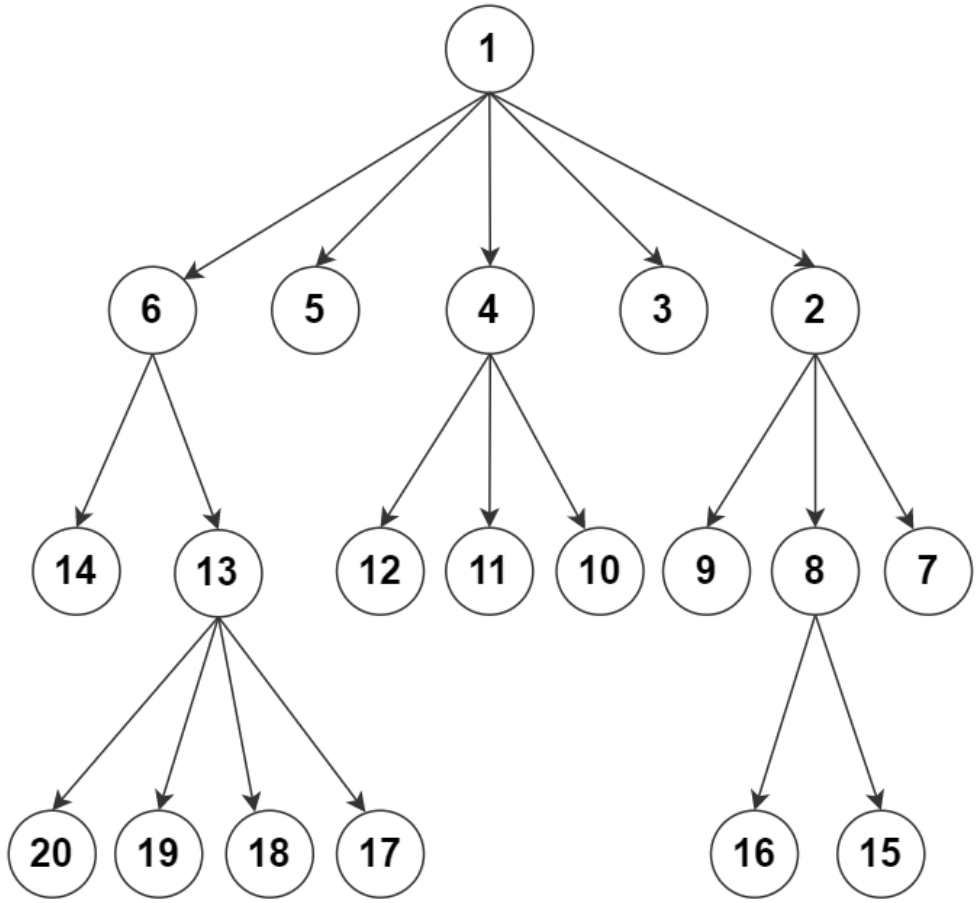


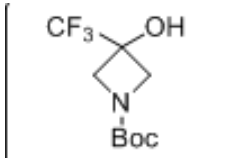
Koscher et al., 2023: https://www.science.org/doi/10.1126/science.adi1407

Limited examples of clinical success with signs of potential

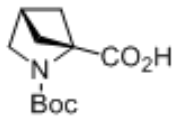
- A handful of examples of Investigational New Drug (IND) filings with early clinical trials
  - These are small molecules
- More examples of de novo drug design showing on target potency and promising pharmacokinetic/safety profiles
  - Likely still challenges with modeling complexity in human biology
  - Potential improvements with better omics measurements to stratify patient population
- Antibody redesign to restore potency is generating impact
  - De novo design still requires further work
- Improvements in protein folding prediction are opening up potential for new de novo biologics design
  - Added potential for peptide design

Traditional chemical search methods do not scale well

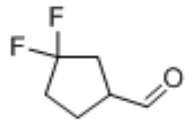




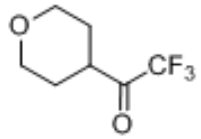
EN300-89728



EN300-27230



EN300-345189



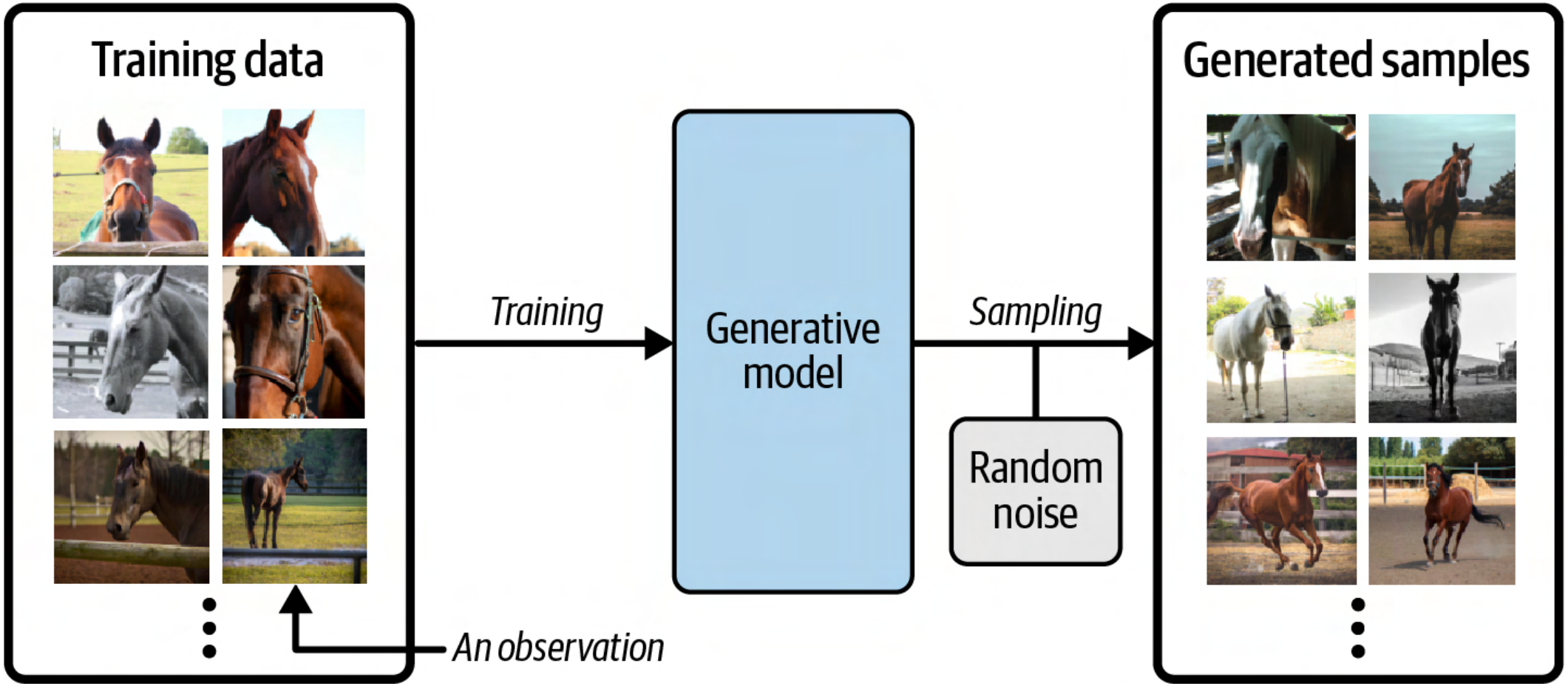
EN300-383280

EN300-106635

Chemical building blocks for compound synthesis

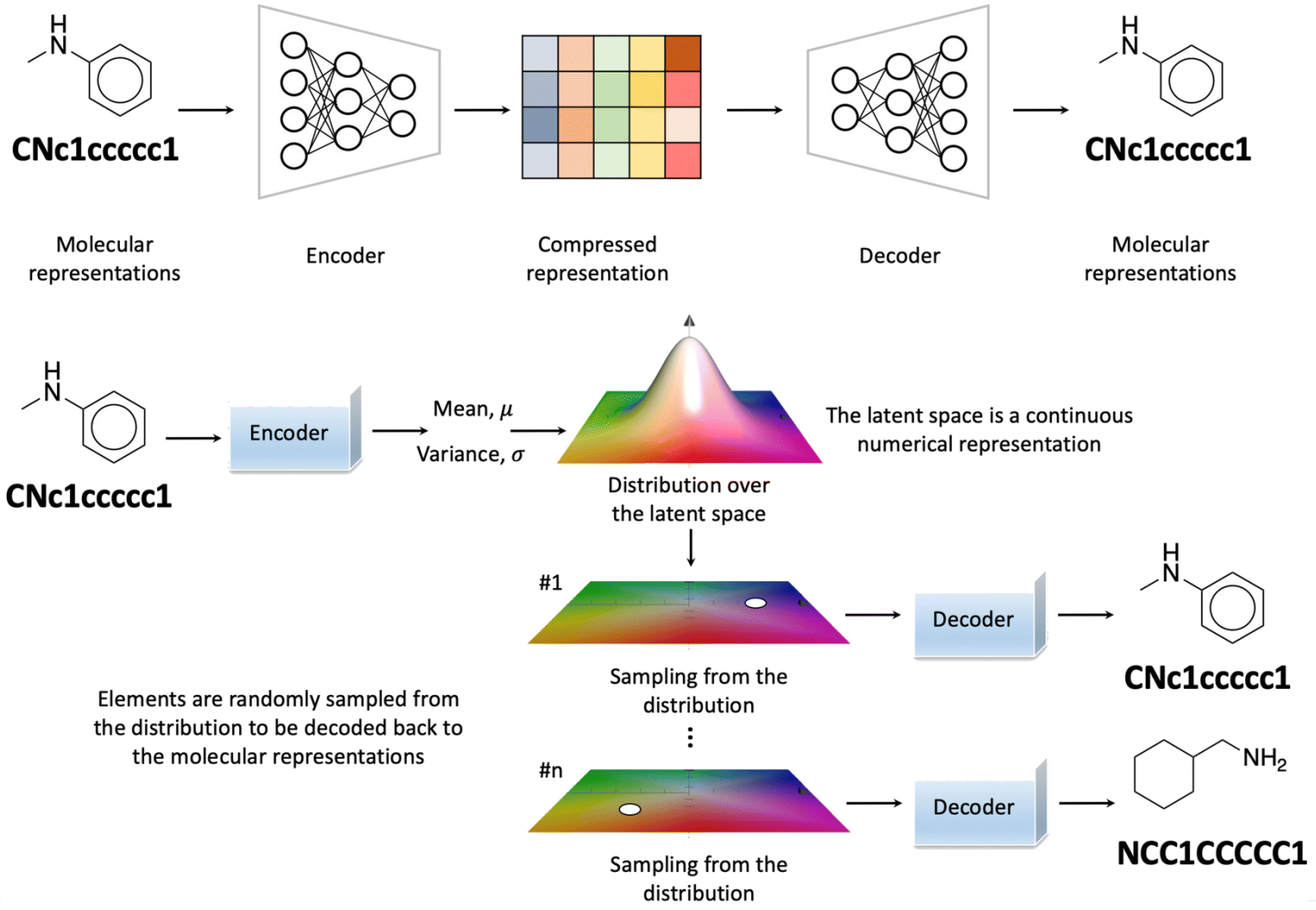
100K+ building blocks ad growing!

Generative molecular models similar to models in other domains

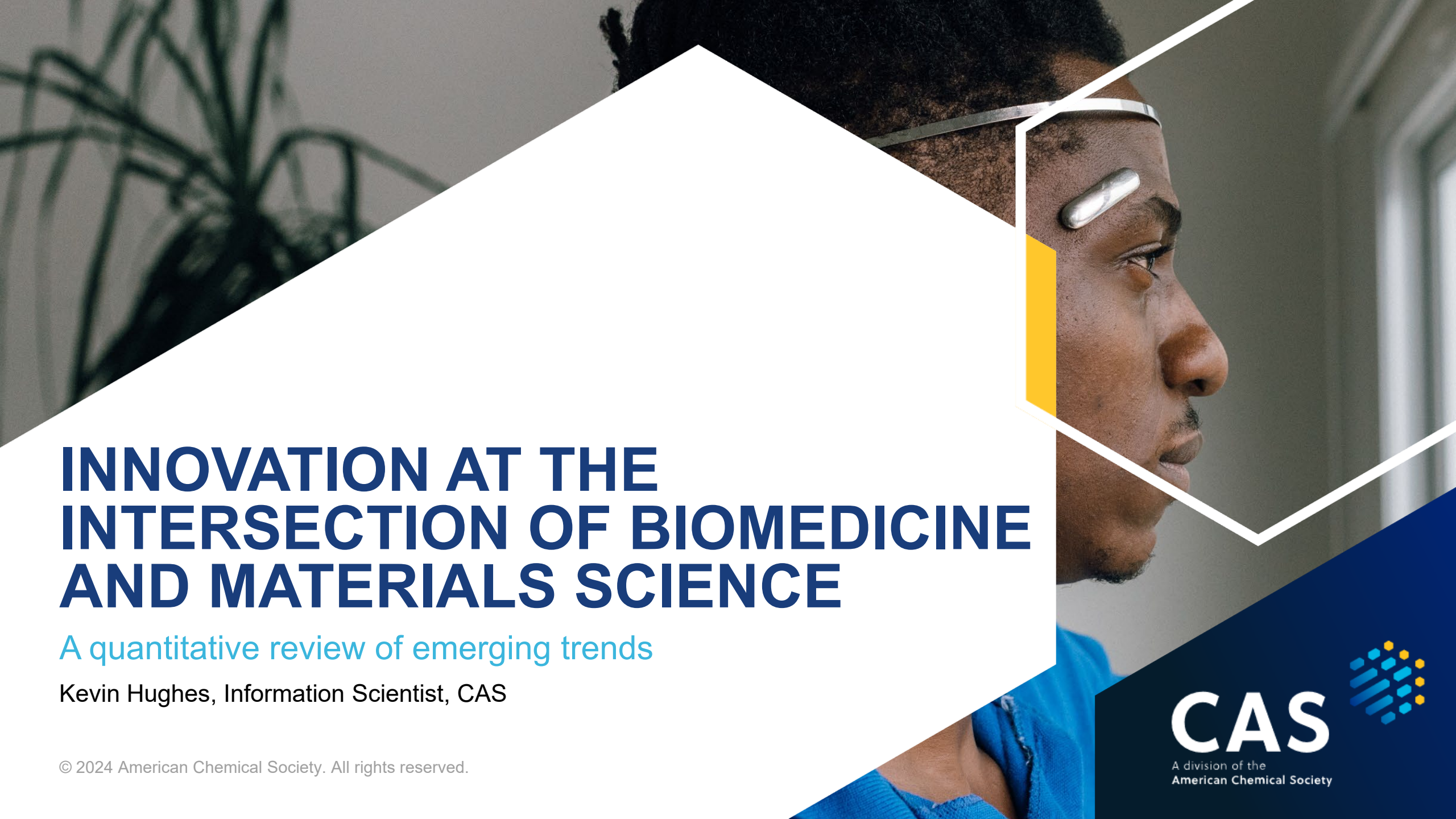


https://www.oreilly.com/library/view/generative-deep-learning/9781098134174/ch01.html

Generative chemical model search larger chemical spaces



Bian and Xie 2021, JMM



INNOVATION AT THE INTERSECTION OF BIOMEDICINE AND MATERIALS SCIENCE

A quantitative review of emerging trends

Kevin Hughes, Information Scientist, CAS

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Identifying top growing trends in biomaterials

Through quantitative data analytics

Key take-aways:

- Innovation is often found at the intersection of disciplines

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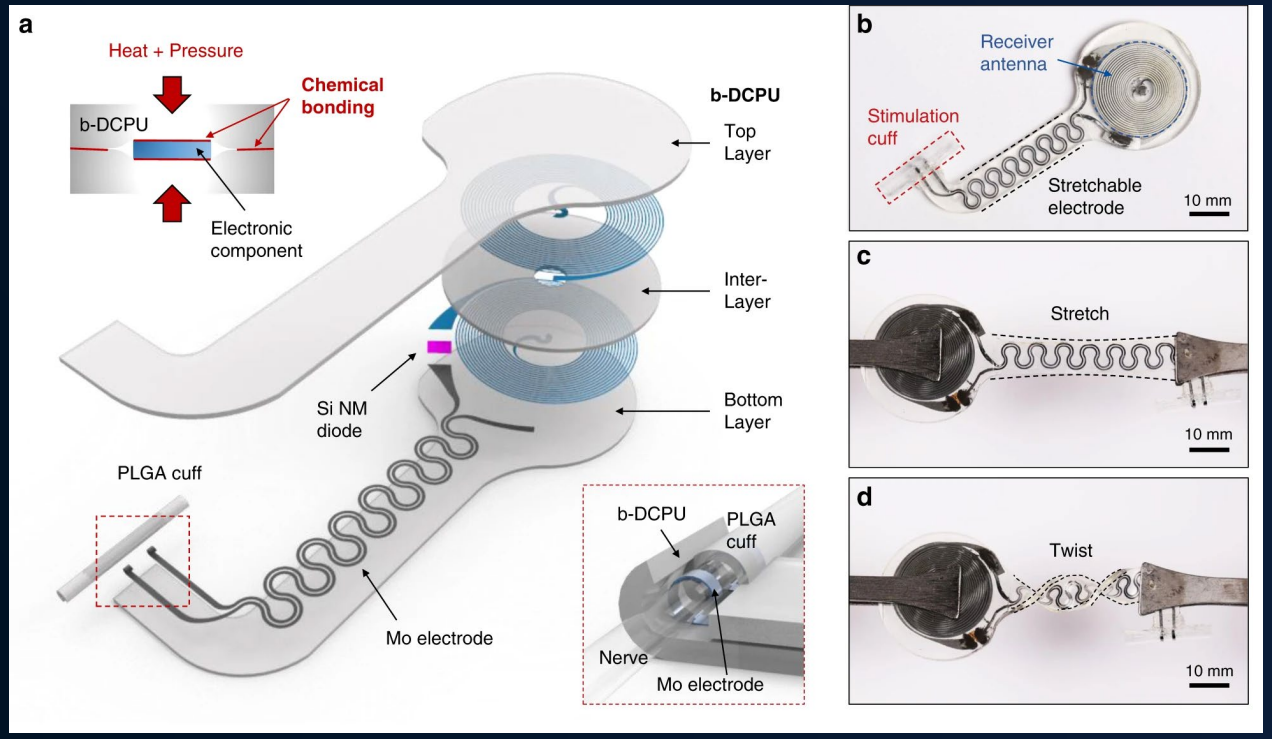

Choi, Y. S., et al. Stretchable, dynamic covalent polymers for soft, long-lived bioresorbable electronic stimulators designed to facilitate neuromuscular regeneration. *Nature Communications* **2020**, *11* (1), 5990

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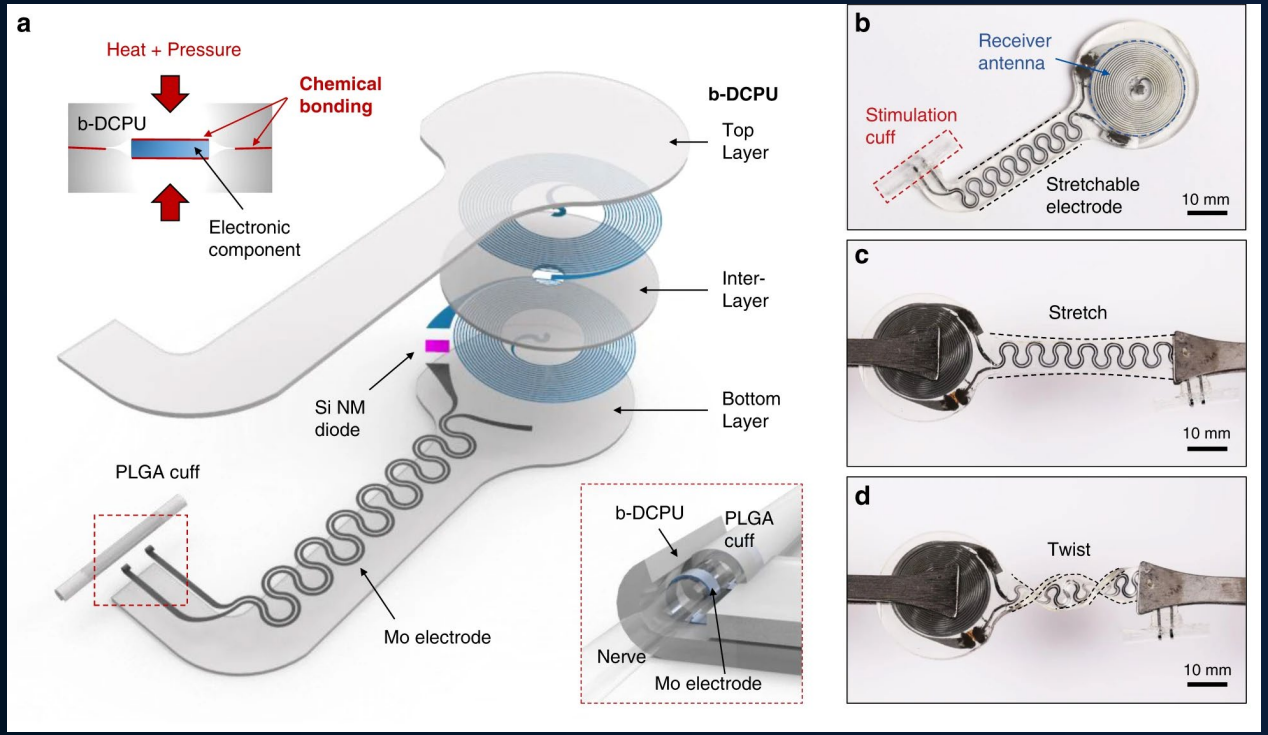
Identifying top growing trends in biomaterials

Through quantitative data analytics

Key take-aways:

- Innovation is often found at the intersection of disciplines
- Goal of this analysis: provide data-based support for decision making and R&D planning



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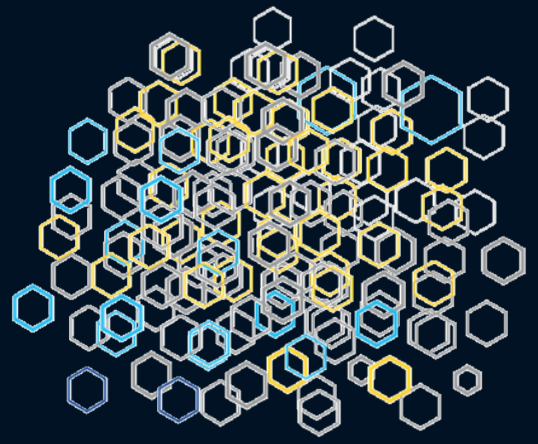
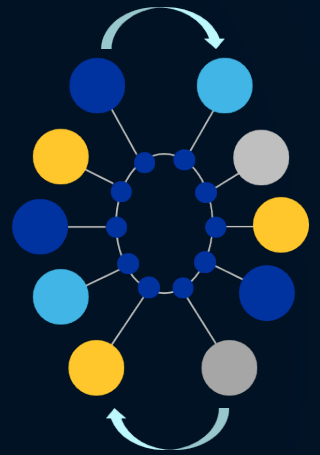
Identifying Emerging Trends

Natural Language Processing (NLP) with SME guidance on large data sets

Query CAS Content Collection to select journal and patent publications in biomaterials

Natural Language Processing (NLP) to identify concepts





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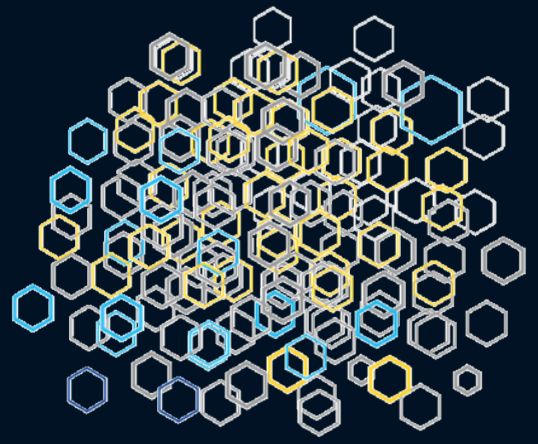
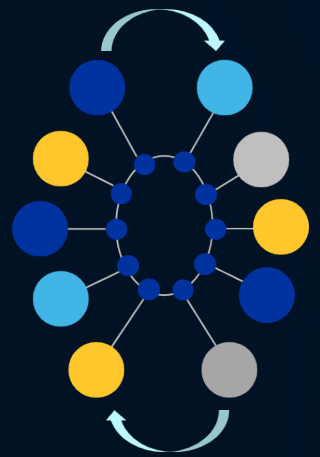
SME review of concepts

Refine





NLP-identified concepts also scored using:

- Publication rate
- Relative growth rate
- Citations

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Natural Language Processing (NLP) with SME guidance on large data sets

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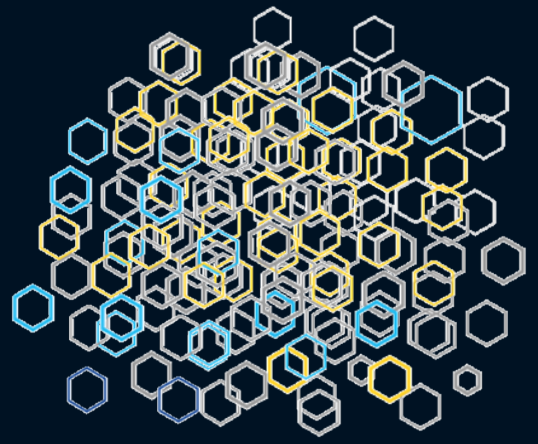
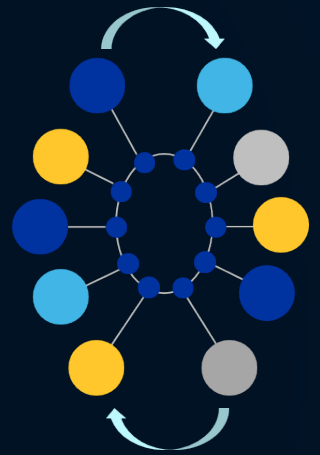
SME review of concepts

Refine

Final topic areas grouped, defined, and further analyzed





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Eight key areas emerged in 3 key categories

Fastest areas of growth, validated by SME expertise into data

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Material Functions

- Programmable biomaterials
- Self healing biomaterials

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- Protein based materials
- Lipid based materials

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Eight key areas emerged in 3 key categories

Fastest areas of growth, validated by SME expertise into data

Material Functions

- Programmable biomaterials
- Self healing biomaterials

Compositions

- Protein based materials
- Lipid based materials

Applications

- Bioinks
- Bioelectronic materials
- Antibiotic materials
- Sustainable alternatives for biomedical materials

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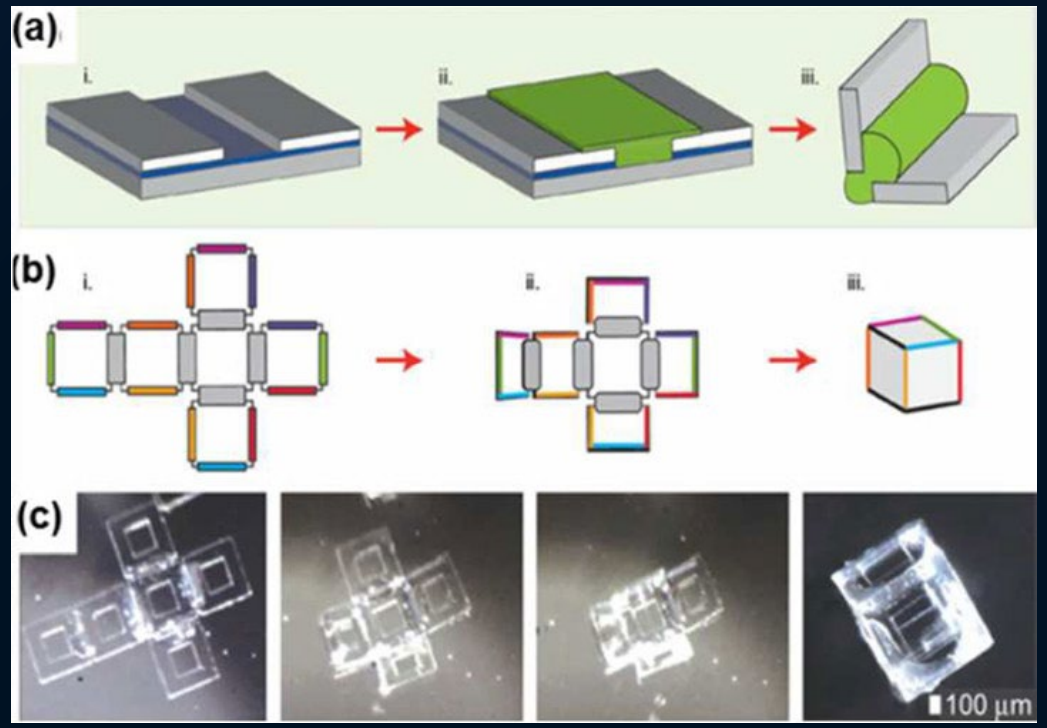
Programmable biomaterials

Stimulus type is a key aspect



Azam, A., et al. Self-folding micropatterned polymeric containers. *Biomed Microdevices* **2011**, *13*(1), 51-58

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Programmable biomaterials

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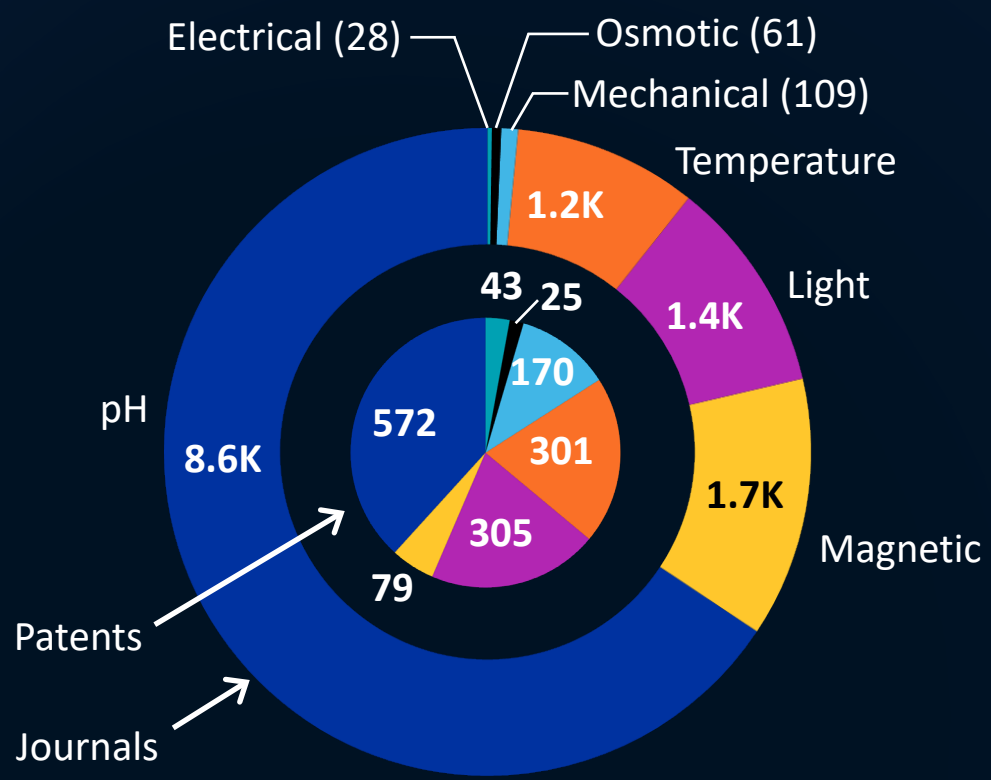

Trend Analysis:

- pH and magnetic stimuli appear more prominently in journal publications
- Mechanical and temperature-based stimuli appear relatively more in patents

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For more details visit cas.org/biomaterials

Dr. Kevin Hughes
Information Scientist
khughes@cas.org

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Trends in Battery Energy Storage

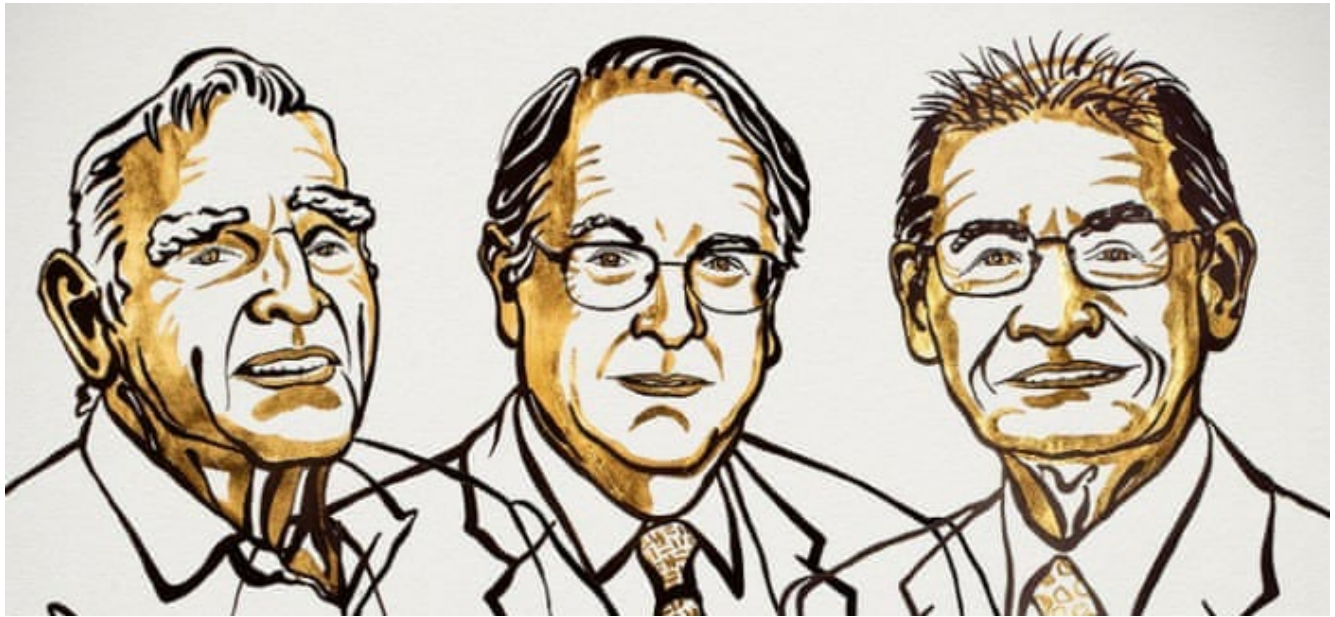
Yiying Wu

Department of Chemistry & Biochemistry
The Ohio State University
Columbus, Ohio

Fifty years of lithium-ion batteries and what is next?

M. Stanley Whittingham* and Jie Xiao

– *MRS Bulletin* **48**, 1118–1124 (2023).



Cell Chemistry

- Li metal anode.
- Solid-state batteries.
- Sodium and potassium-based batteries.
- Extreme Conditions.
- Sulfur batteries.
- Oxygen batteries

Beyond the Cell Chemistry

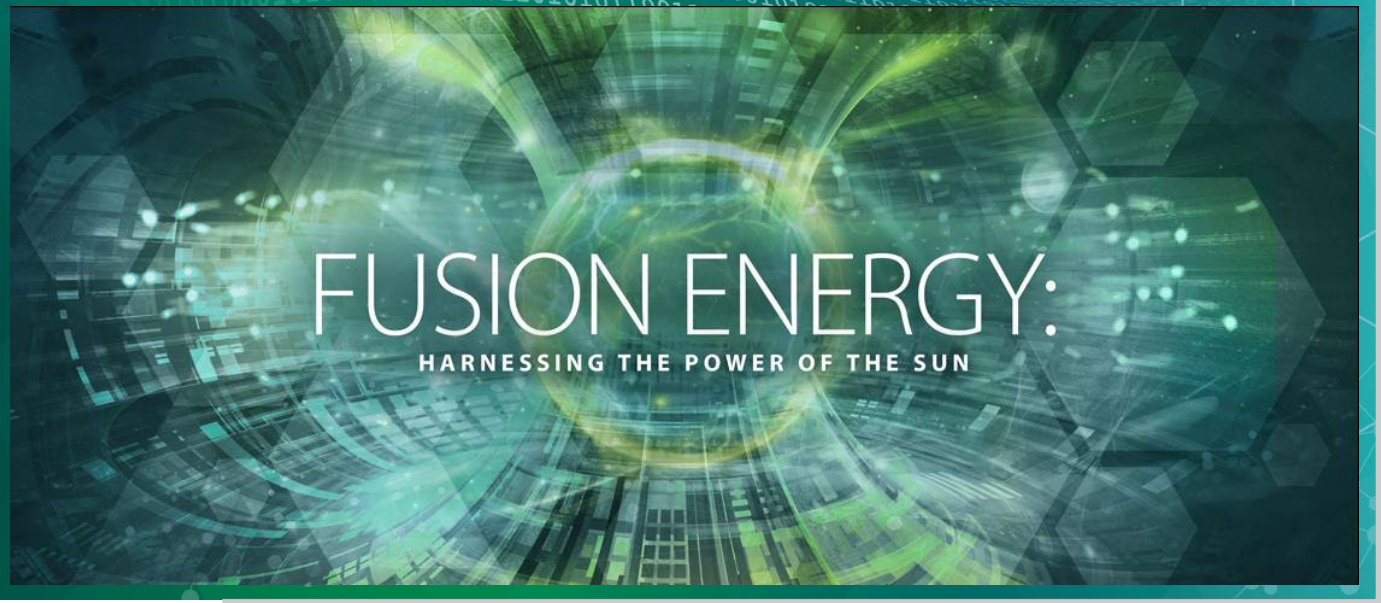
- - Manufacturing technologies for batteries: reducing energy consumption and transportation costs.
- - Regional supply chains and clean mining with renewable energy.
- - From Cradle to Cradle: Recycling for reducing waste and recovering materials from end-of-life batteries.
- - Safety is a big concern, and overdesigning safety into materials and systems is necessary.

OAK RIDGE National Laboratory

~~Nuclear~~ Fusion Energy

Arnold Lumsdaine
Director, Innovation Network for Fusion Energy (INFUSE)
Oak Ridge National Lab

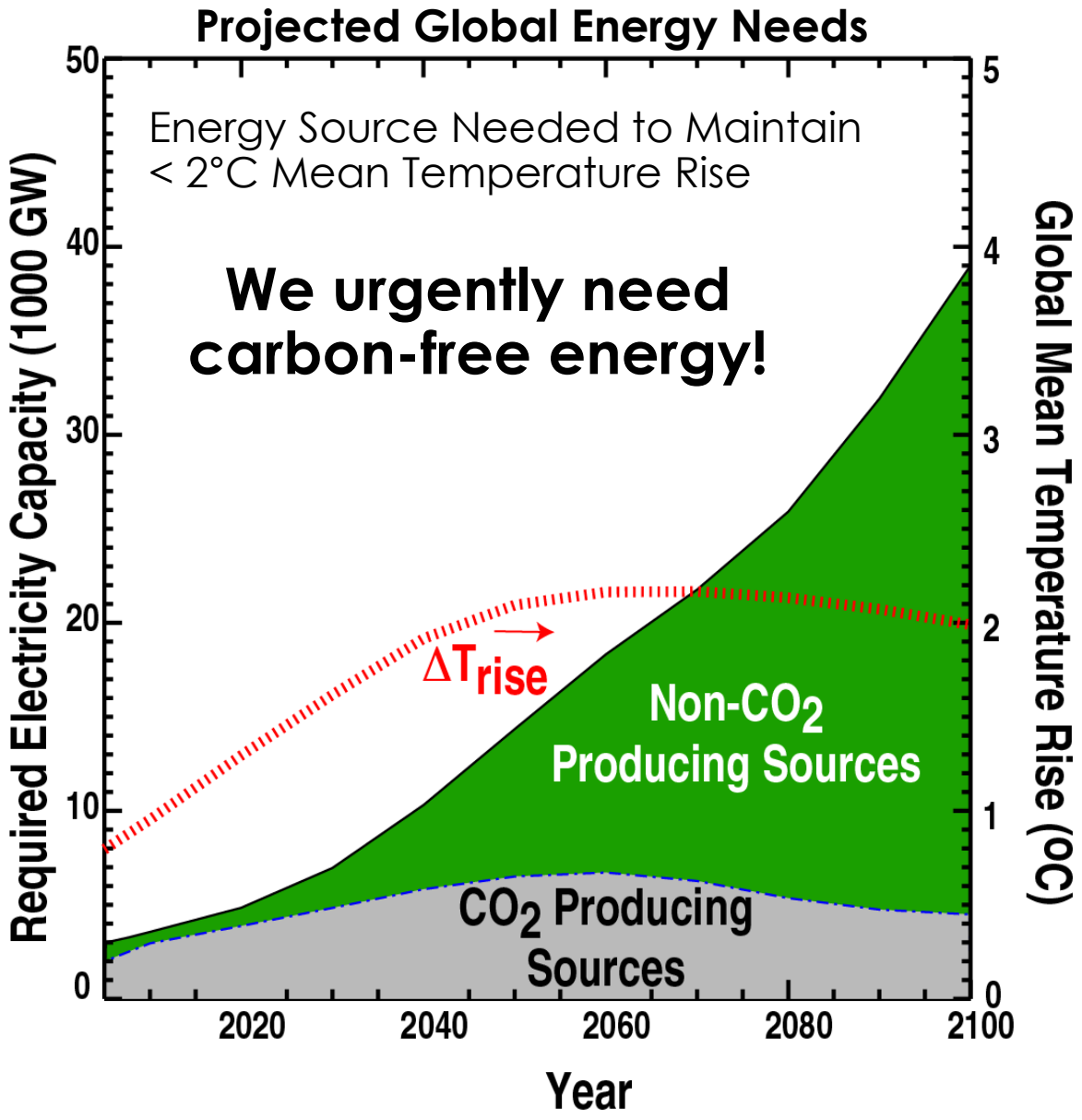
January 25, 2024



ORNL is managed by UT-Battelle, LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

The Future of Our Civilization Depends on Energy



Source: IPCC AMPERE Project, AMPERE-450-FullTech-OPT Scenario

- Projected need for ~ 35,000 GW from non-CO_2 producing sources

35,000 1 GW-e plants !!!

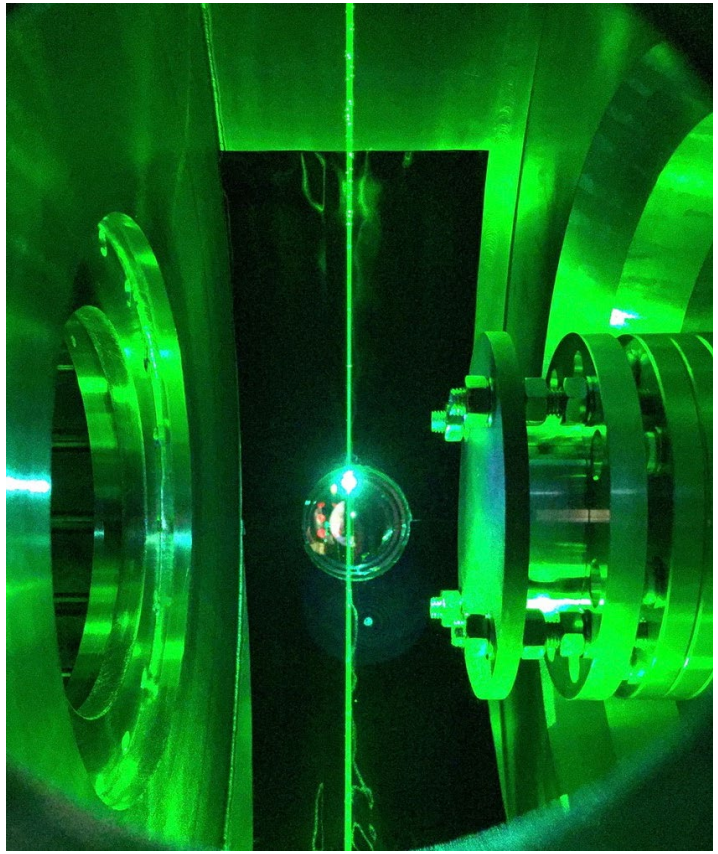
- By 2050, annual global energy investment would need to reach $0.66 T ($23 T cumulative)
  - GDP (2018): US: $21T, China: $14T, UK: $2.9T
  - Global cell phone market: $0.55 T

Source: IRENA, Global energy transformation, 2019

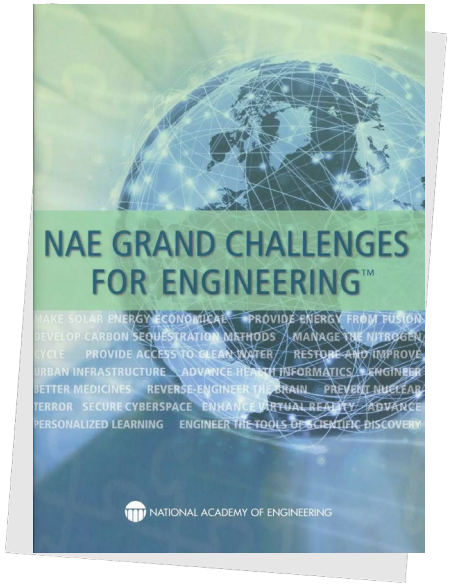
A New Era in Fusion Energy Development Has Dawned

Confluence of developments have positioned fusion for a major 20-year push

- Achievements on National Ignition Facility and Joint European Torus demonstrate fusion energy production
- Multiple reports for U.S. expert groups indicate readiness and urgency of fusion development
- Extensive predictive tools for optimizing performance now in place
- New technologies available to address key challenges
  - Superconductors, Materials by Design, Advanced Manufacturing, High Performance Computing
- Significant escalation in investment in clean energy → new $$$ to make push possible



The National Academies says that it's time

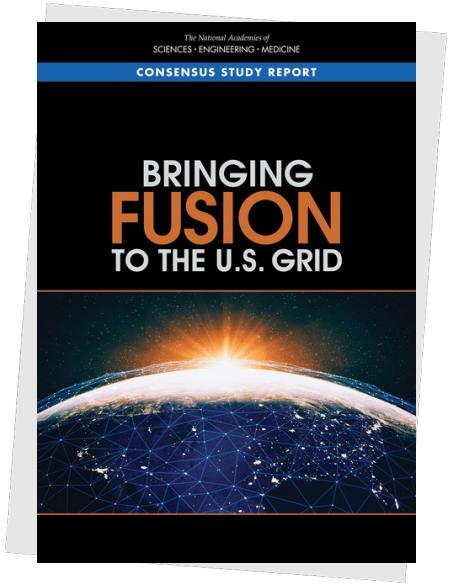


NAE (2017)

Identified "Provide energy from fusion" as a grand challenge for the 21st century

NASEM (2018)

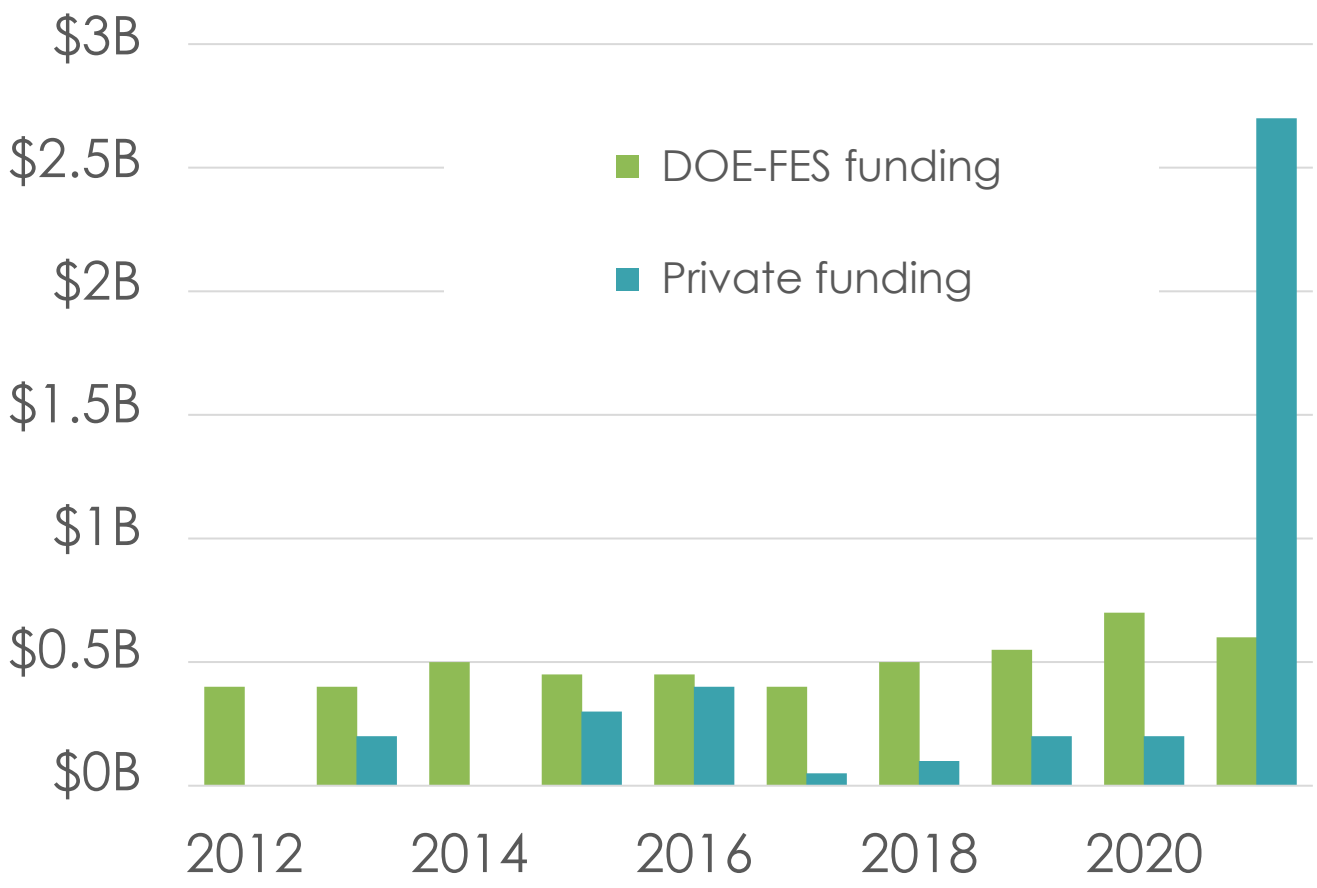
"Now is the right time for the United States to develop plans to benefit from its investment in burning plasma research and take steps towards the development of fusion electricity for the nation's future energy needs"



NASEM (2021)

"Successful operation of a pilot plant in the 2035–2040 timeframe requires urgent investments by DOE and private industry—both to resolve the remaining technical and scientific issues and to design, construct, and commission a pilot plant."

Private investment in fusion has surged in recent years



Currently over $6B invested

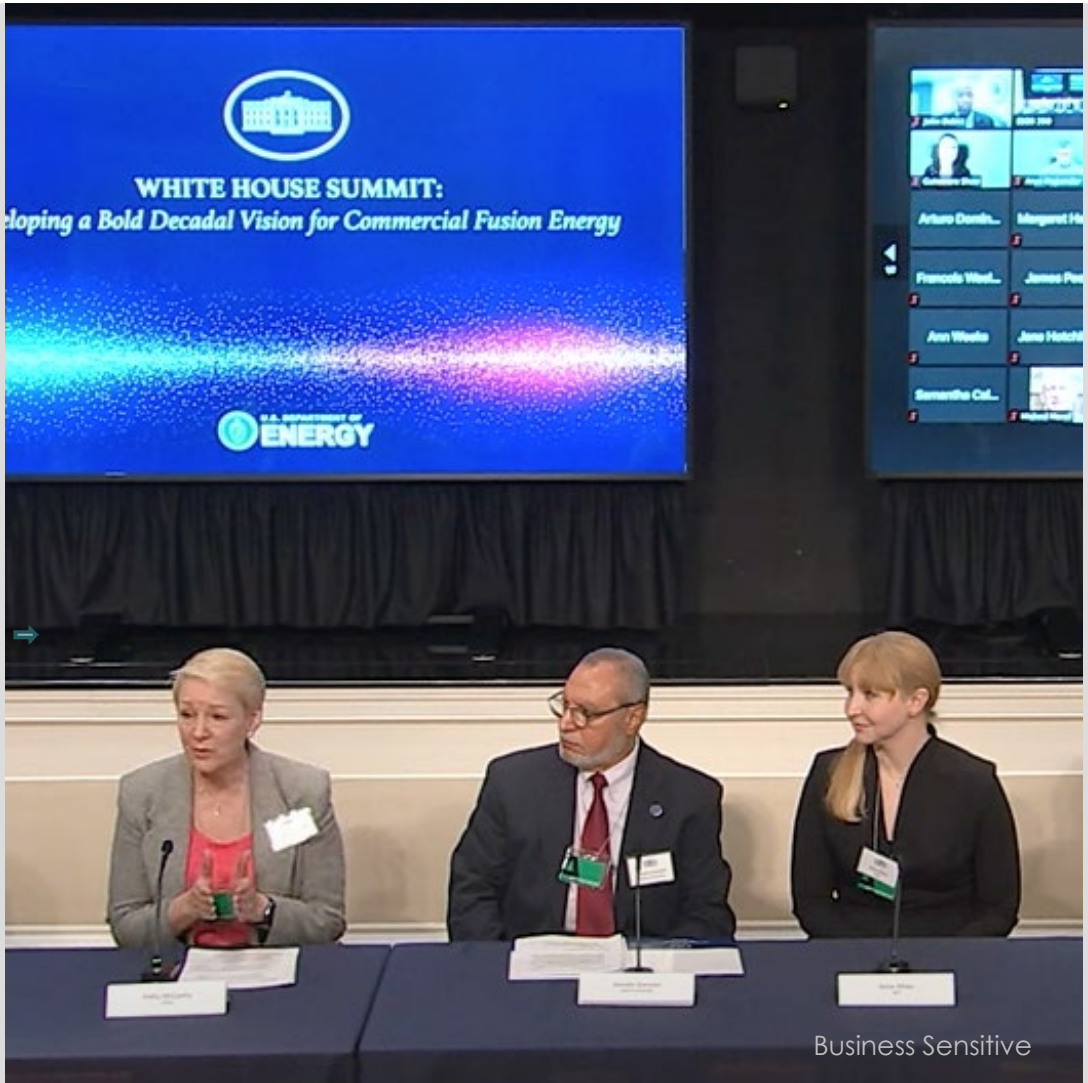
https://www.fusionindustryassociation.org/news/from-the-fia/#industry-reports

US government has announced a decadal initiative to develop fusion energy

White House Summit on Developing a Bold Decadal Vision for Commercial Fusion Energy

"Fusion is a potential carbon-free, abundant source of clean energy that will bolster American leadership, strengthen energy security, and enable sustained energy independence"

Rep. Chuck Fleischmann (TN)



US ITER Project Director Kathy McCarthy speaking during the White House summit on March 17, 2022

Department of Energy Focus on Public-Private Partnerships

INFUSE program

- Enables private firms to tap into national lab and university resources to address key issues
  - Led by ORNL and PPPL https://infuse.ornl.gov/

11 Participating DOE labs

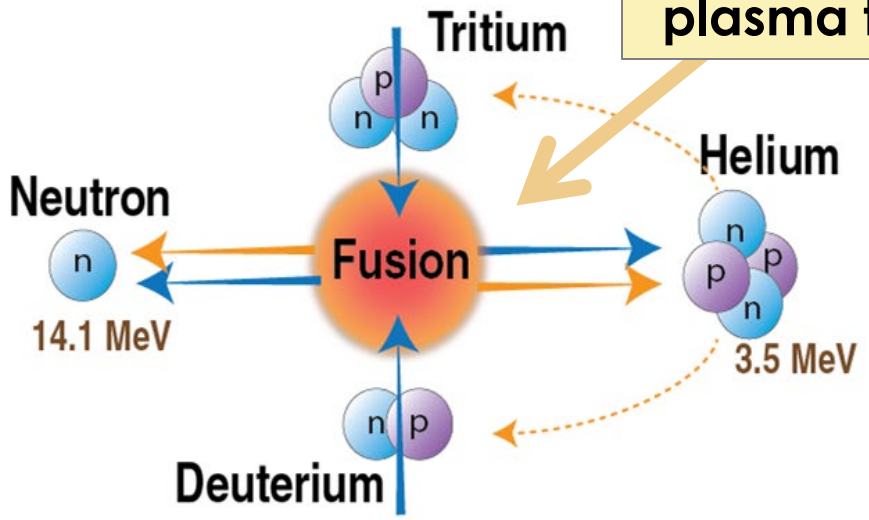
Fusion Industry Association

Milestone Program

- In 2023, the DOE Office of Fusion Energy Sciences launched a milestone-based fusion development program, with $46M for private companies (with 50% cost share) towards the development of fusion power with completion of preliminary design expected within 5 years.
- Eight awards were announced:
  - Commonwealth Fusion Systems
  - Focused Energy, Inc.
  - Realta Fusion
  - Thea Energy
  - Tokamak Energy
  - Type One Energy
  - Xcimer Energy Corporation
  - Zap Energy

Generating Electricity from Fusion Energy Requires Meeting Three Scientific/Technological Challenges

<u>Control, sustain, and predict</u>
a high temperature "burning" plasma to produce neutrons/heat



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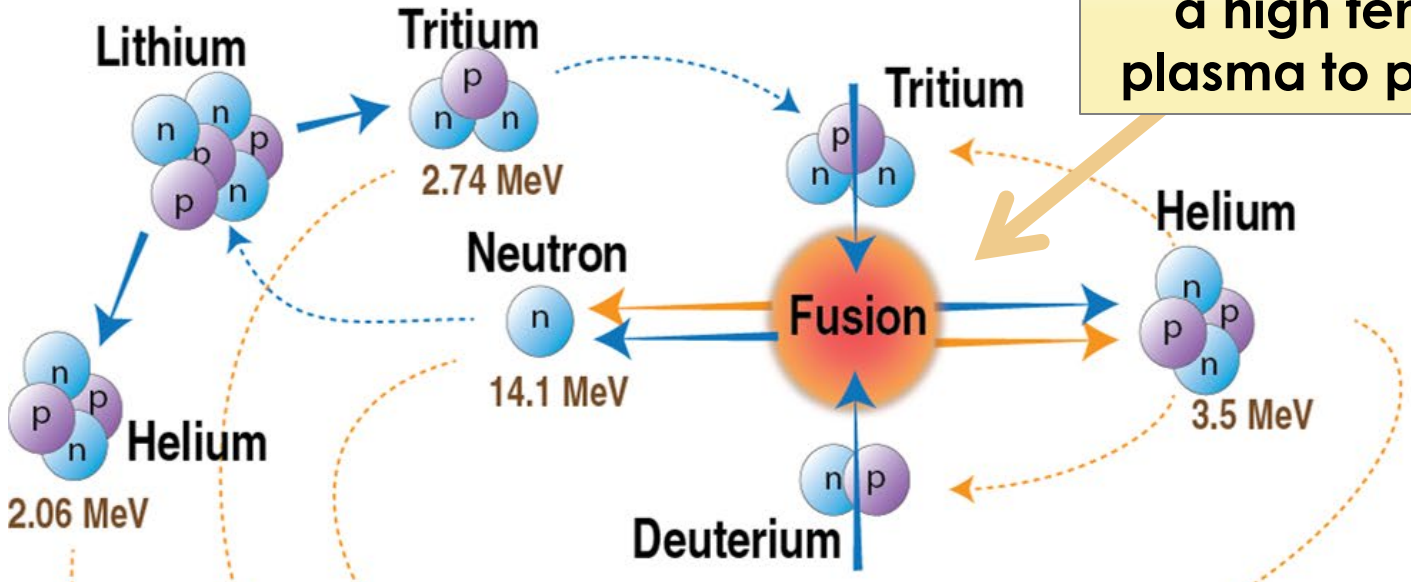

<u>Find materials</u>
that can handle extreme conditions of reactor

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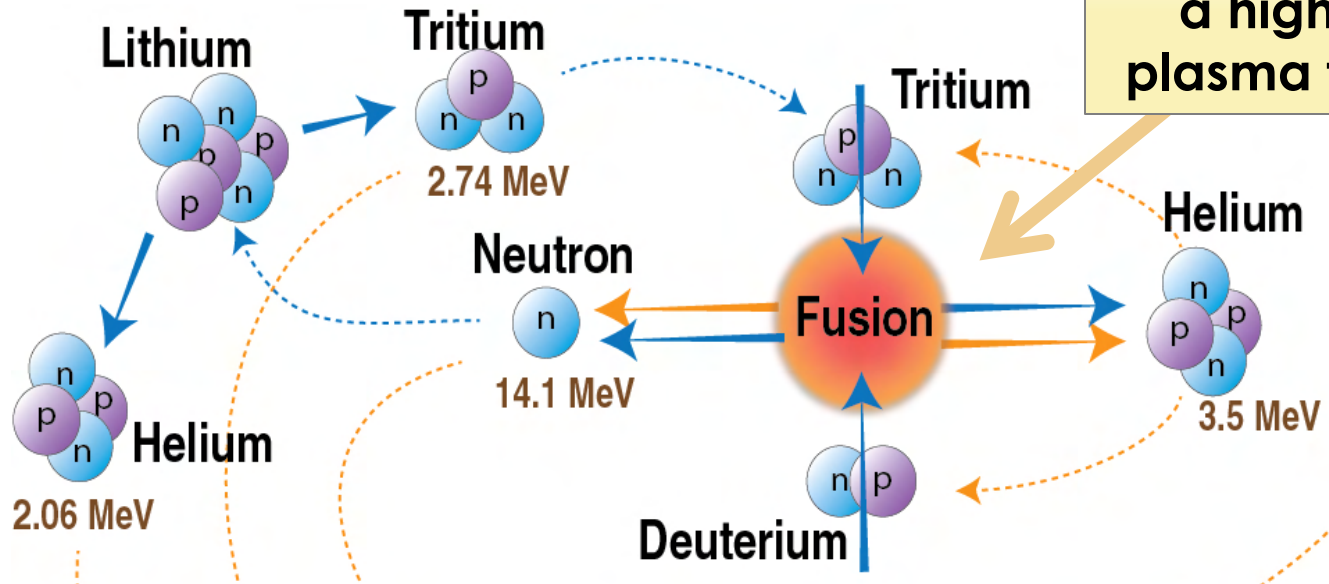

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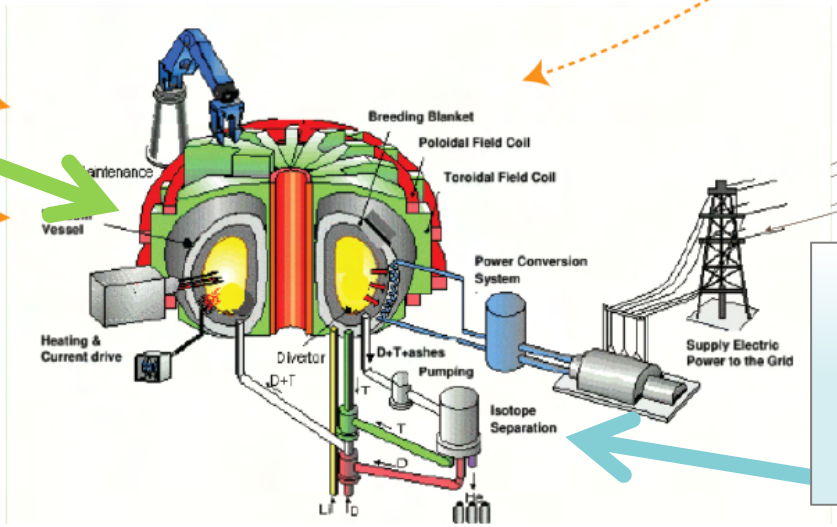


Particle Flow

Energy Flow

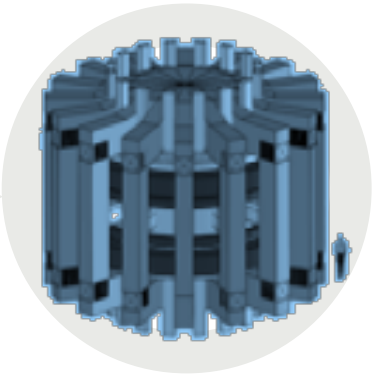
Harness fusion power
by capturing the energy, breeding sufficient tritium, and reliably producing net electricity

Technical readiness must be advanced rapidly to meet ambitious timelines for fusion implementation

Creating and sustaining a fusion power source

Materials to survive in the fusion environment

Fuel self-sufficiency and harnessing fusion power



Fusion pilot plant

Imaginable Plausible Feasible Practical

Technical Readiness Level (TRL)

1 2 3 4 5 6 7 8 9

Approximate technical readiness today

Materials challenges are complex involving multiple extremes

Cottant et al., 2008

Hydrogen embrittlement

High Temperature & High Stress

Transmutation-assisted corrosion

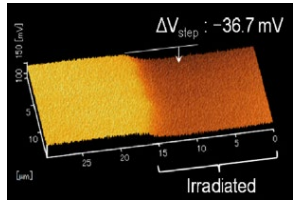
Stress-corrosion cracking

Irradiation/transmutation-assisted corrosion

Chemical Environment

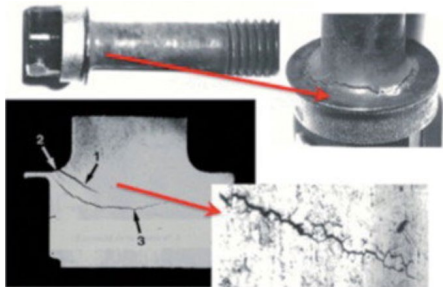
Irradiation-assisted corrosion

Atomic Displacement



Kondo et al., 2016

Irradiation-assisted stress-corrosion cracking



Allen et al., 2010

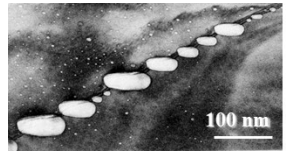
Irradiation/transmutation-assisted stress-corrosion cracking

Helium-assisted cavity swelling

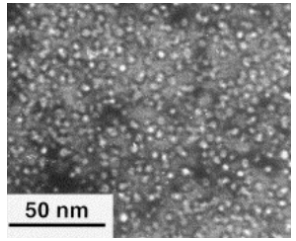
Irradiation-creep, fatigue, embrittlement

Transmutations

High-temperature helium embrittlement



Braski et al., 1979

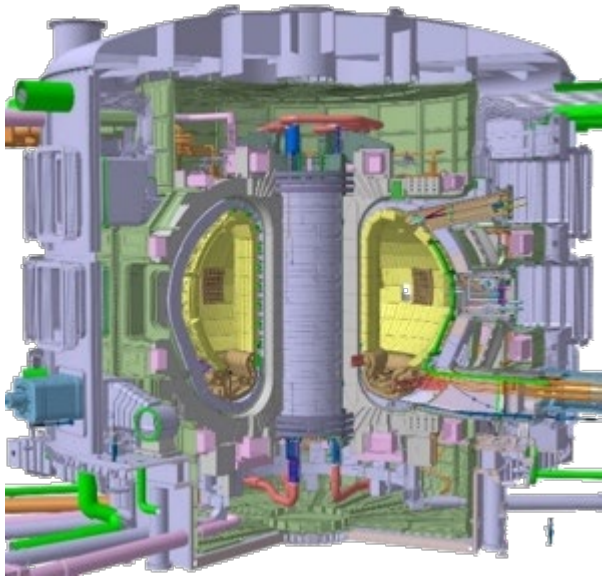


Chernov et al., 2003

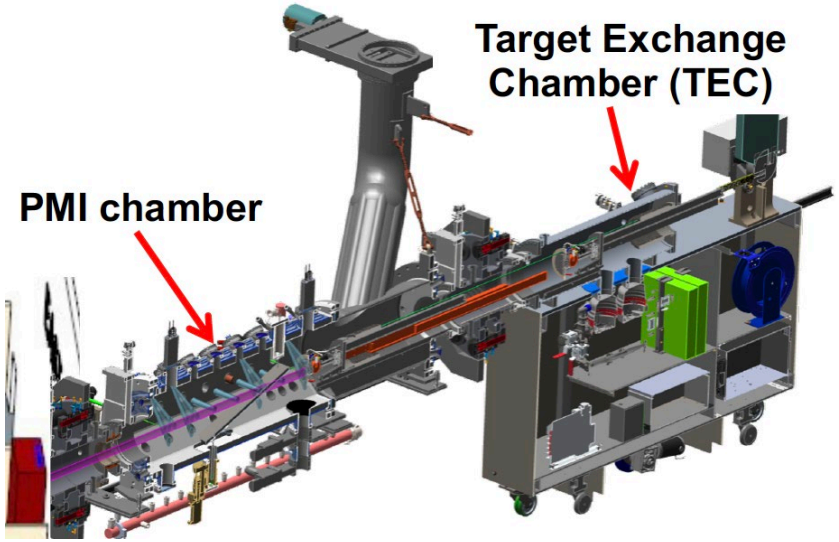
Fusion Facilities in the Next Decade

- **ITER** is a 35-nation collaboration under construction in Cadarache, France, and is expected to produce 500 MW fusion power for 400s, and begin operation in the 2030's.
- The **MPEX** project will the support the development of candidate plasma facing materials and is currently under construction, with operation expected in early 2028.
- A **Fusion Prototypic Neutron Source** has been identified by the fusion community as a critical next facility to fill critical material science gap for exposure to fusion neutrons.

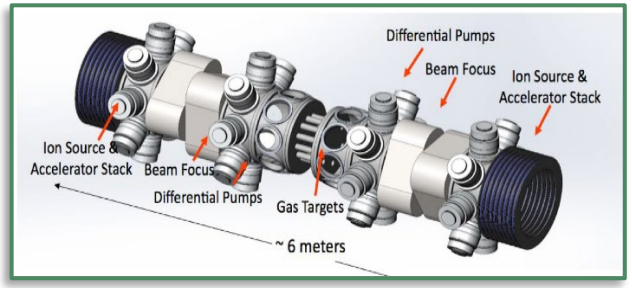
ITER



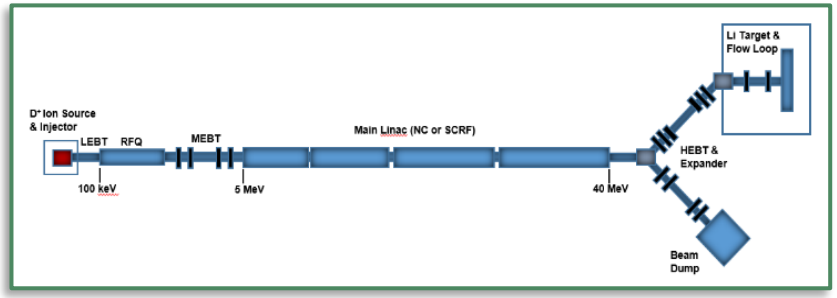
MPEX



Multibeam D^+ into T gas target fusion neutron source



D – Li stripping reaction ~5 MW D accelerator and liquid Li target



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