Using AI to accelerate scientific discovery

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PCAST

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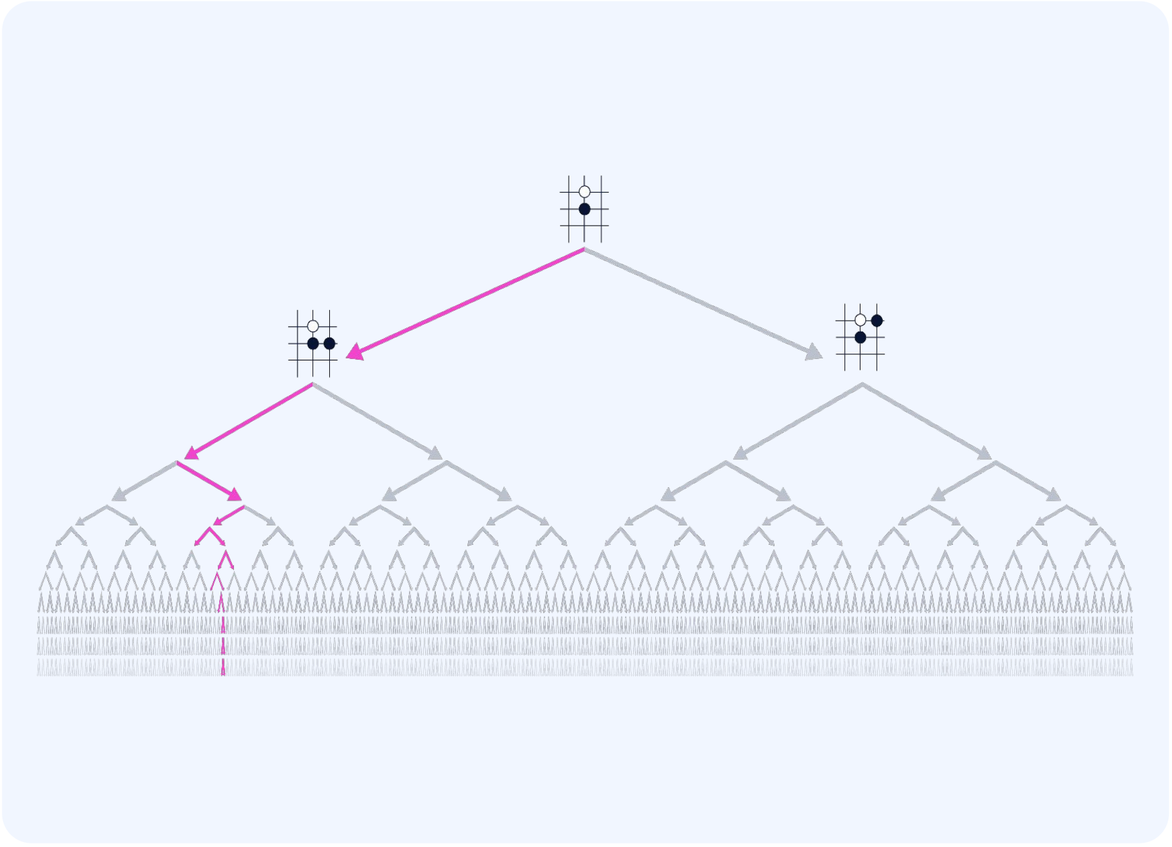
Google DeepMind

AI breakthroughs in games laid the foundation for scientific applications

AlphaGo - mastering Go through self-learning



Guiding the search with the model

The Protein Folding Problem

AMINO ACID SEQUENCE

3D PROTEIN STRUCTURE

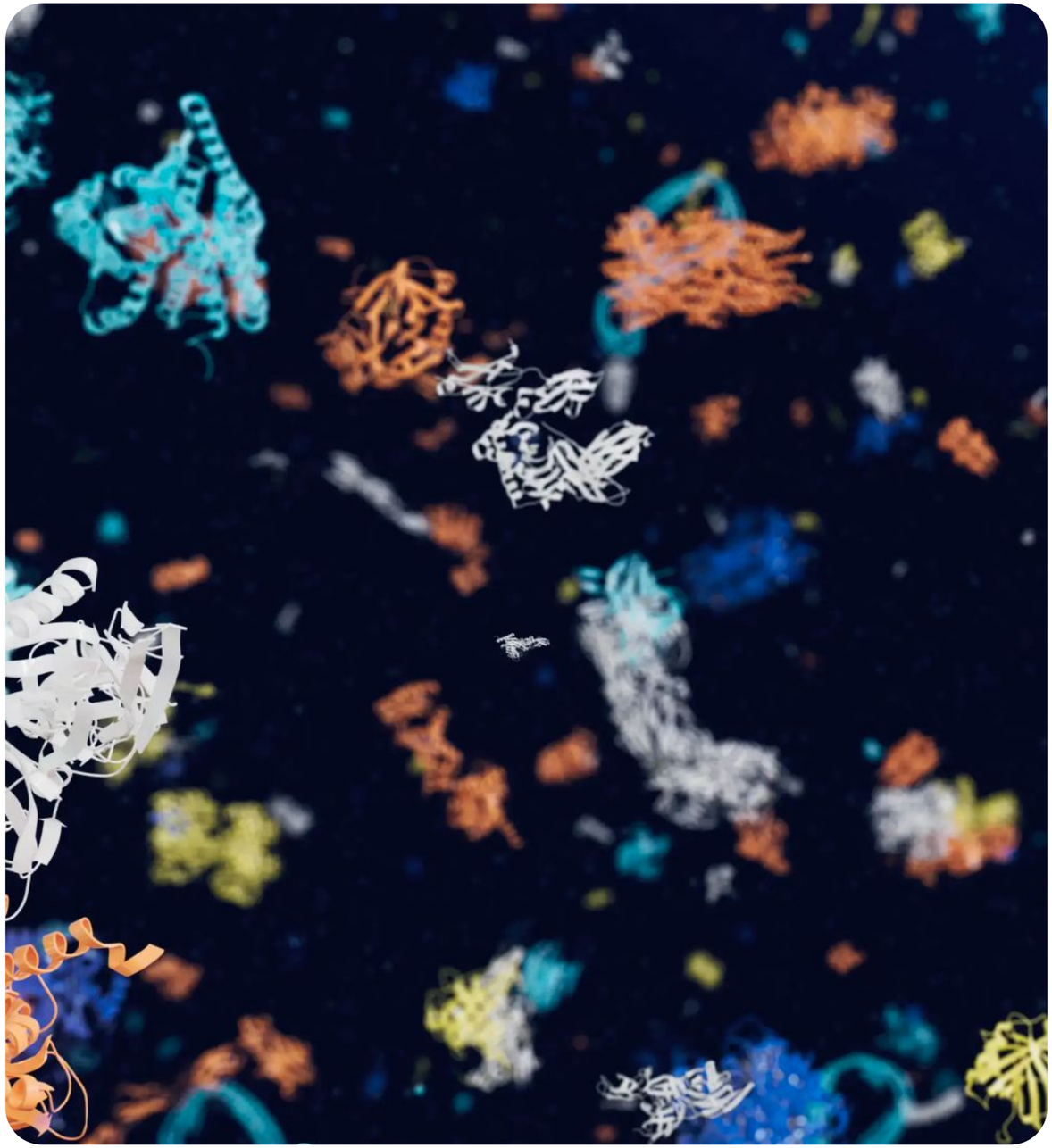
Proteins are essential to all life - their function partially depends on their 3D structure

Determining the structure often takes years of painstaking experimental work

“The 3D structure of a protein… should be fully determined by the amino acid sequence”

Christian Anfinsen, Nobel Lecture 1972

A 50-year-old grand challenge in biology



We folded all 200M+ proteins known to science with AlphaFold

All predictions are freely available in the AlphaFold Protein Structure Database

1M+ users

190+ countries

10000+ citations

~1B years of PhD time

AlphaFold is accelerating progress on a range of important problems

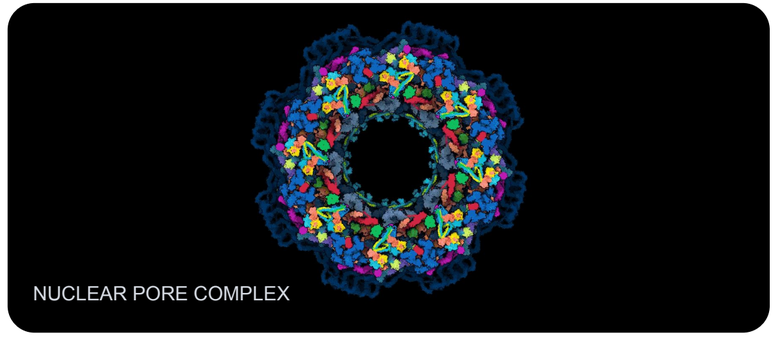
See more **#Unfolded** stories at **unfolded.deepmind.com**

Plastic pollution

Designing plastic eating enzymes
McGeehan et al. (Portsmouth)

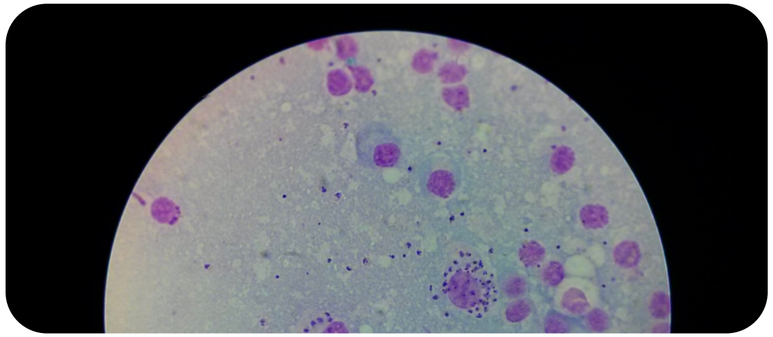
Antibiotic resistance

Blocking antibiotic resistance mechanisms
Sousa & Mitchell (Colorado)



Structural biology

Determined structure of nuclear pore complex
Fontana et al., Mosalaganti, et al. (Science)



Neglected diseases

Accelerating drug discovery in Leishmaniasis
Benjamin Perry (DNDi)

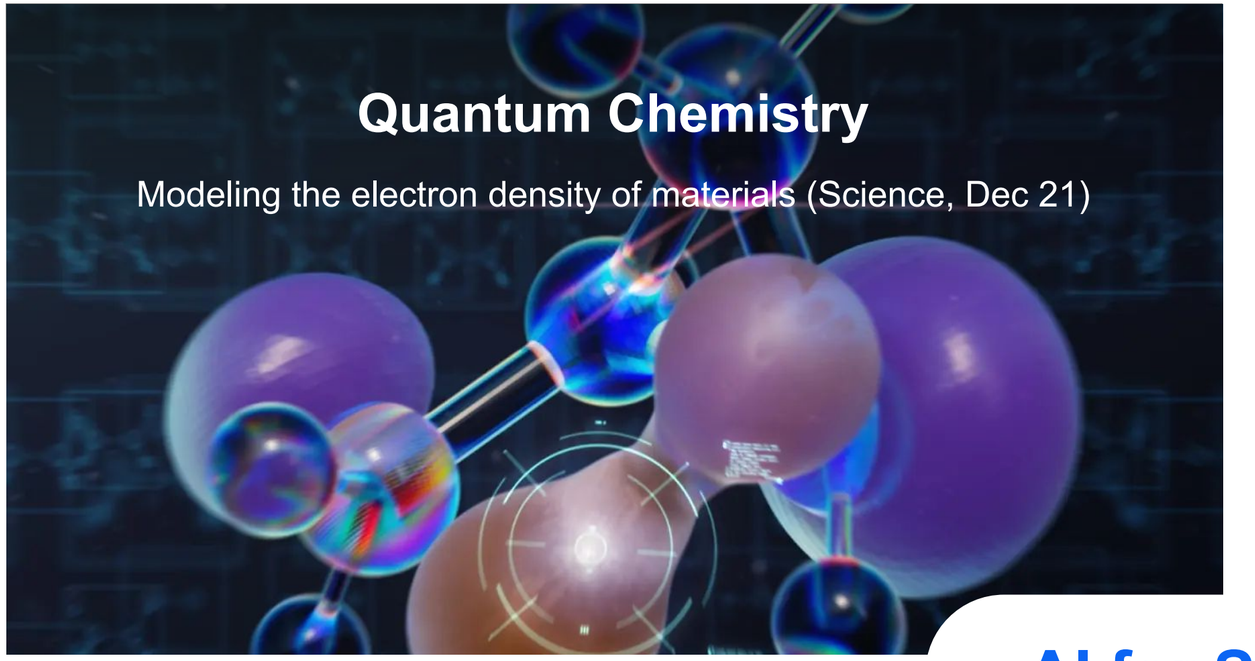
Malaria vaccine

Designing a more effective malaria vaccine
Matthew Higgins (Oxford)

Drug delivery

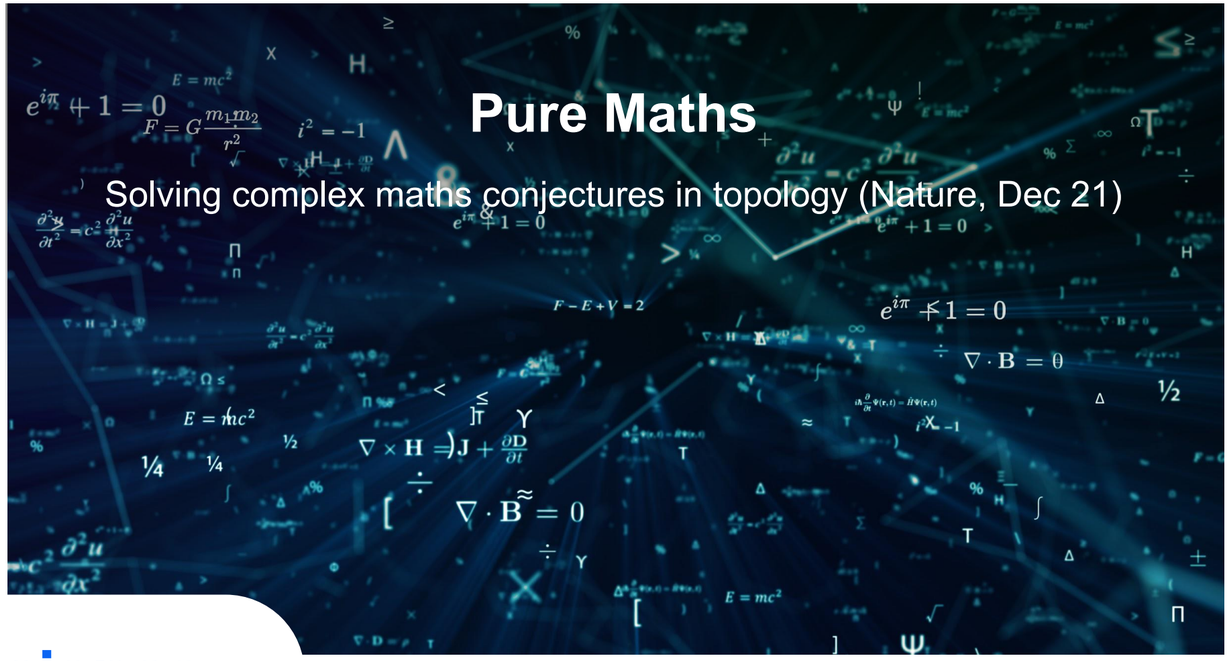
Molecular syringe for protein delivery
Feng Zhang (Broad Institute)

AI for Science



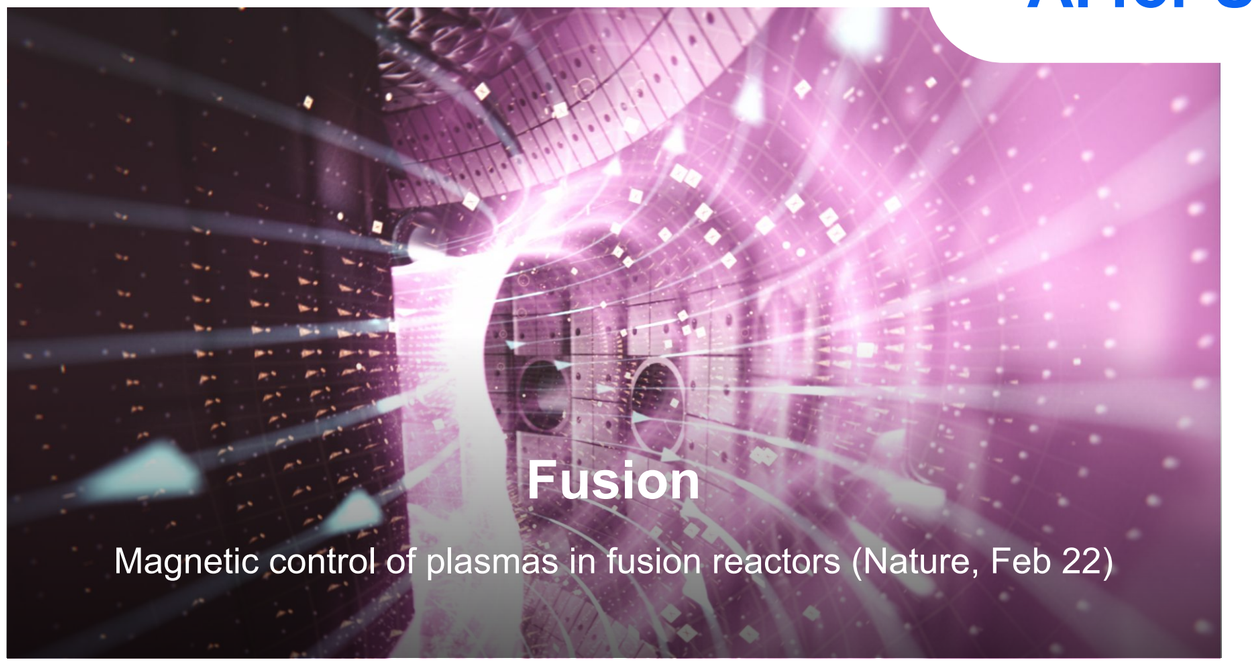
Quantum Chemistry

Modeling the electron density of materials (Science, Dec 21)



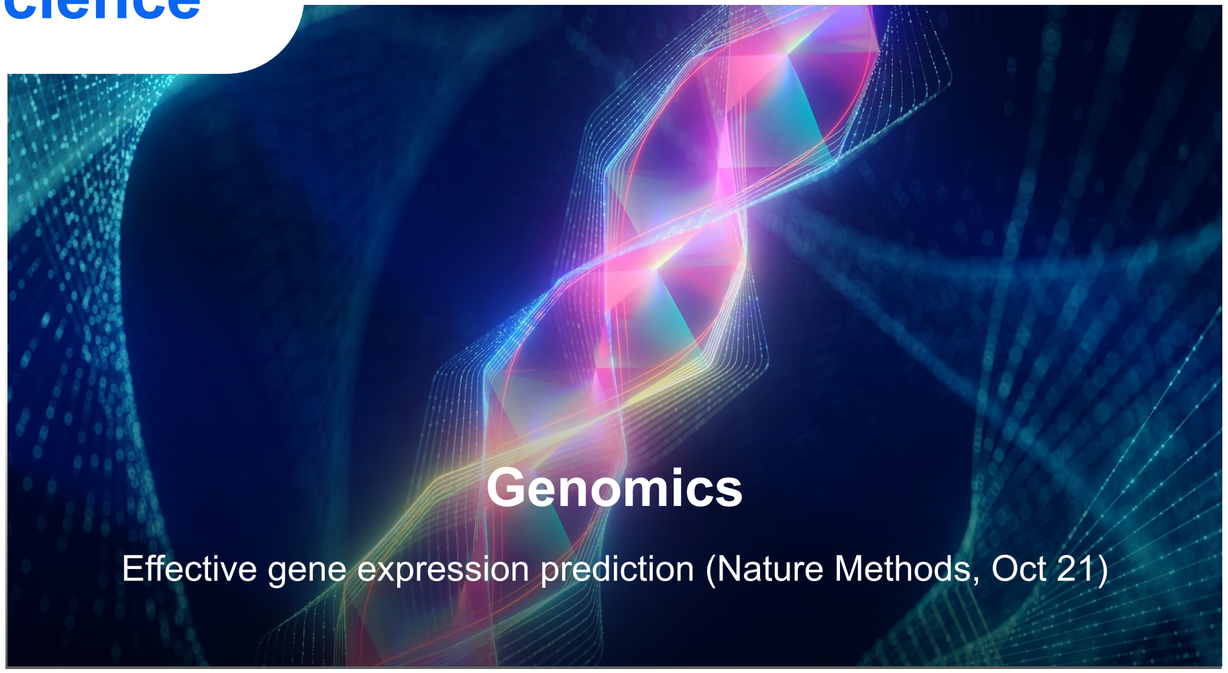
Pure Maths

Solving complex maths conjectures in topology (Nature, Dec 21)



Fusion

Magnetic control of plasmas in fusion reactors (Nature, Feb 22)



Genomics

Effective gene expression prediction (Nature Methods, Oct 21)

Pioneering Responsibly

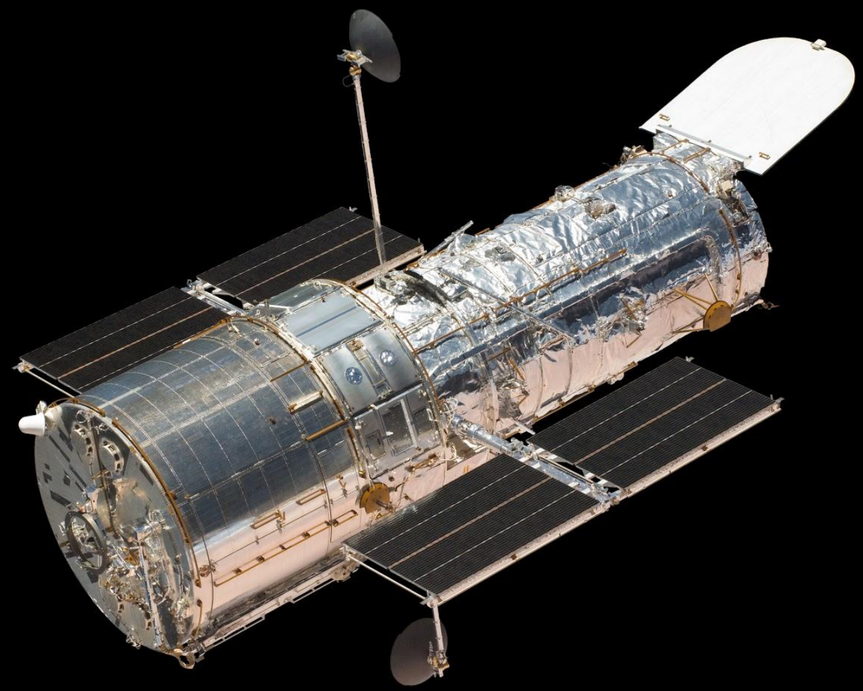
We need to be bold ***and*** responsible. Transformative technology deserves exceptional care

AI has incredible potential to help with humanity's greatest challenges like science and medicine

But AI must be built responsibly and safely, and be used for the benefit of everyone

Ethics and safety has been central to our mission from the beginning - evolved into Google's AI Principles

We continue to provide responsible thought leadership on AI strategy, risks, ethics and safety for the community



AI - the ultimate general-purpose tool
to help us understand the universe