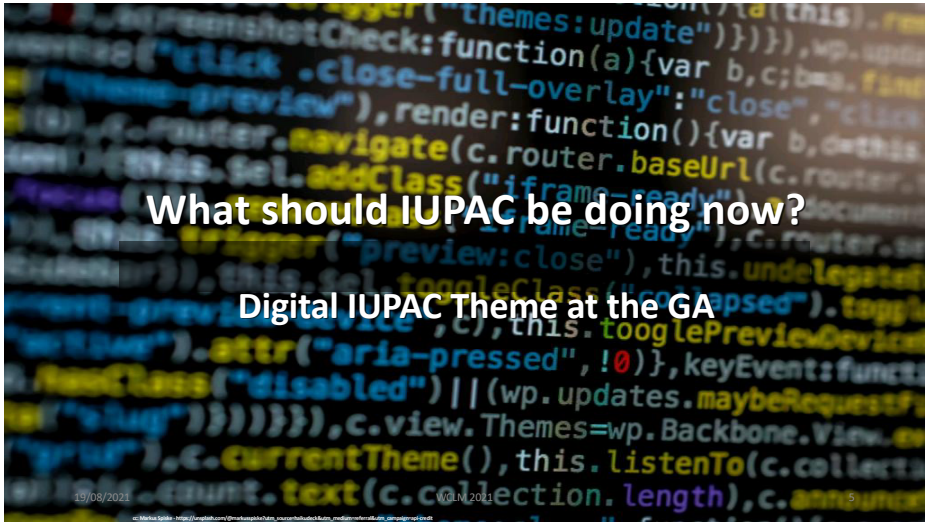
How do we shape the future ?

What are the critical issues to be addressed?

Jeremy G. Frey University of Southampton UK



Applications

devices

materials

crystals

Molecules

mixtures

Drug targets

Personalized medicine

Rare diseases

People and animals

Genomics

Complex formulations

Environment

Machines

Precision agriculture

Engineering

Vastness of chemical Space

- How have we coped so far?
- Inspired by nature!
- Imagination and creativity?

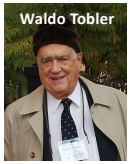
Characterization Techniques

The more of chemical space we plan to explore the more molecules we need to make to provide the data and the less of each molecules we can afford to make.

AI needed to interpret complex measurements

Measurements in context needed – in the cell or device and on the field

https://www.embl.org/news/lab-matters/spc-mosbri/

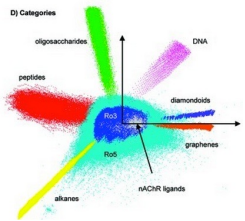


Laws of Geography

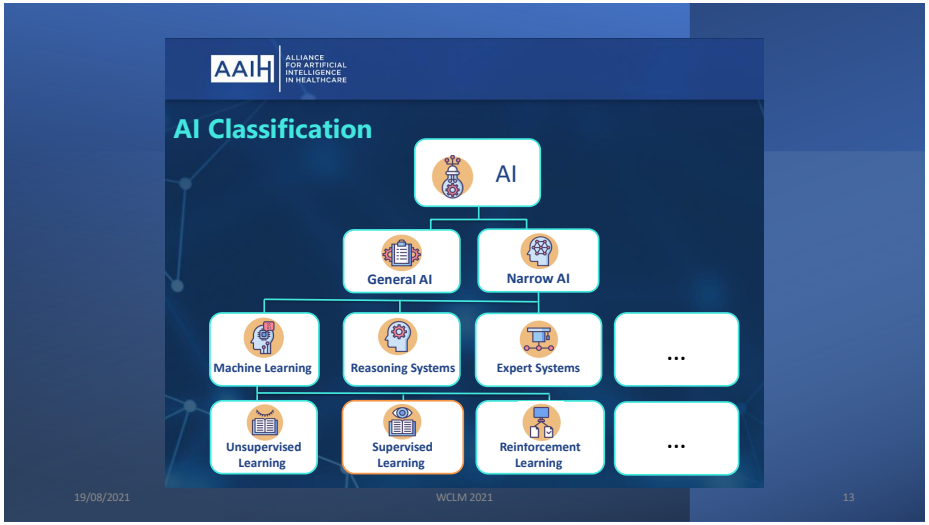
- **The First Law**
  ”Everything is related to everything else, but near things are more related than distant things”.
- **The Second law**
  "The phenomenon external to an area of interest affects what goes on inside".

maps

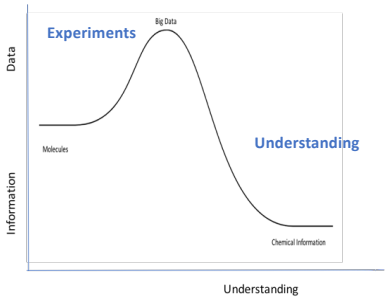
Chemical Space

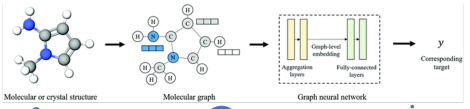


Learning



The more data we have the more we need to throw away





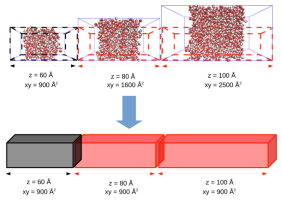
Molecules
Structure
Molecular Graph

Machine Learning
Learn Relevant Descriptors

Chemical Space
Latent Space

Can we get the learning back out of the ML Neural Network?

Machine Learning, Statistical Mechanics & Simulations



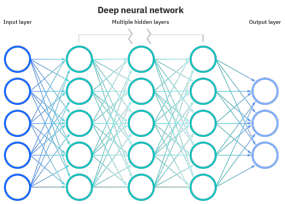
Molecular Dynamics

Develop Force Fields

Faster Integrations

Identify patterns

Enhanced sampling



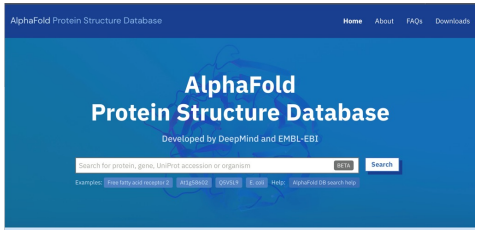
Machine Learning

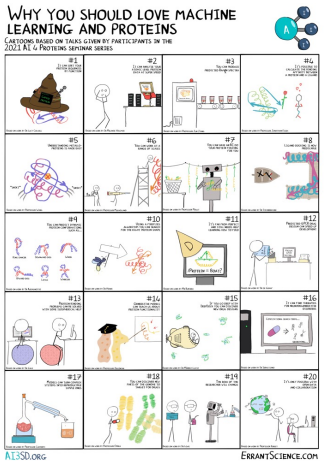
Dynamics

Generative Models

- ML network learns the essential features for molecules with selected properties (e.g., a suitable drug candidate)
- Can be used to select suitable molecules from a library
- But a generative network 'creates' possible molecules
- Then check if there is a synthetic pathway to make them!

Proteins

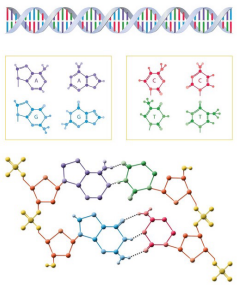


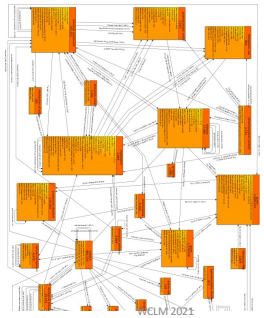


DATA Driven

quantity
quality
uncertainty
provenance
availability
Data revival

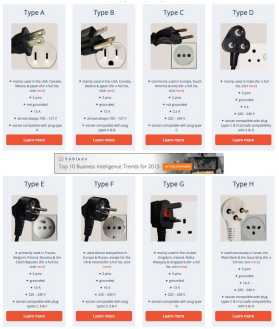
Graphs





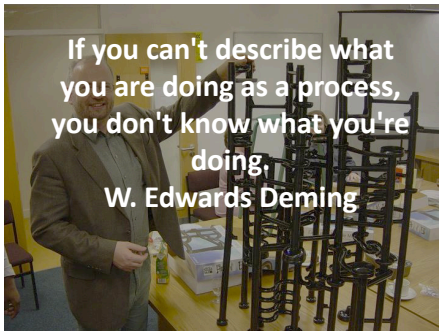
- Molecular Graphs
- Knowledge Graphs
- Graph Neural Networks

Standards – as much time converting as extracting….



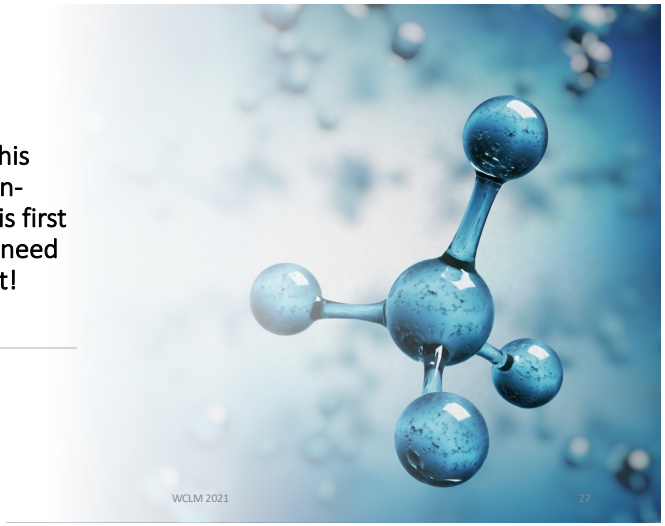
How do we communicate models and process?

- Surprisingly difficult to explain what a process involves
- Much of the detail is assumed to be understood and not explicitly discussed
- This is where the miss-understandings usually arise.

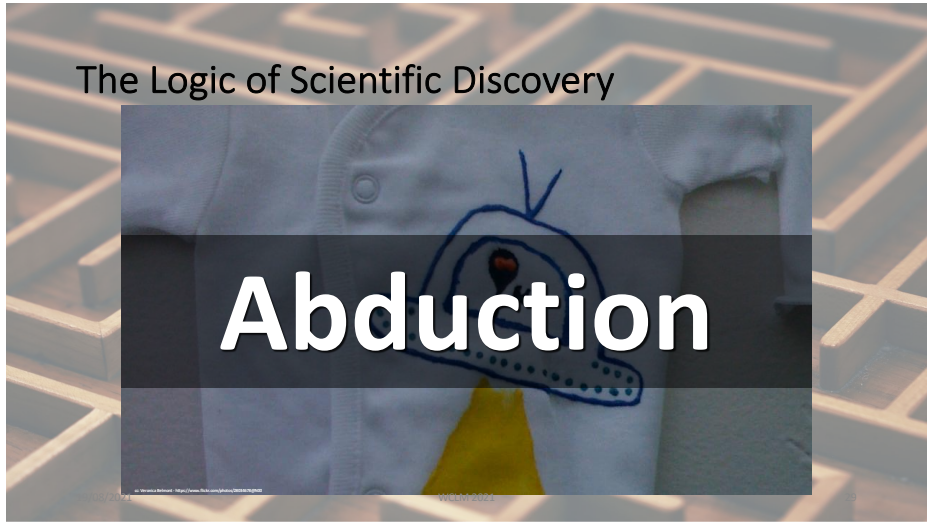


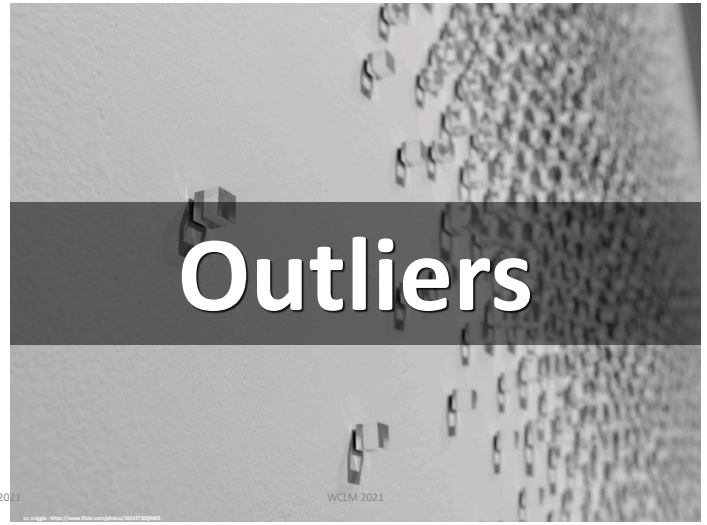
IUPAC must drive this work otherwise non-chemists will do this first – they can see the need even if we have not!

Not a good idea!



https://upload.wikimedia.org/wikipedia/commons/3/38/Perth_Impossible_Triangle.jpg





Finding the Underlying System

Small Data Learning

Include chemical knowledge

Deal with non-linearity

Ethical AI – The Problems of Bias

Explainable
Accountable
Reproducible

All needed for scientific discovery

The Future (is ours to see)

When chemistry becomes a discipline, mathematical chemists will design new materials, predict their properties, and tell engineers how to make them — without ever entering a laboratory. We've got a long way to go on that one!

Robert A. Heinlein, "Where to?" 1950

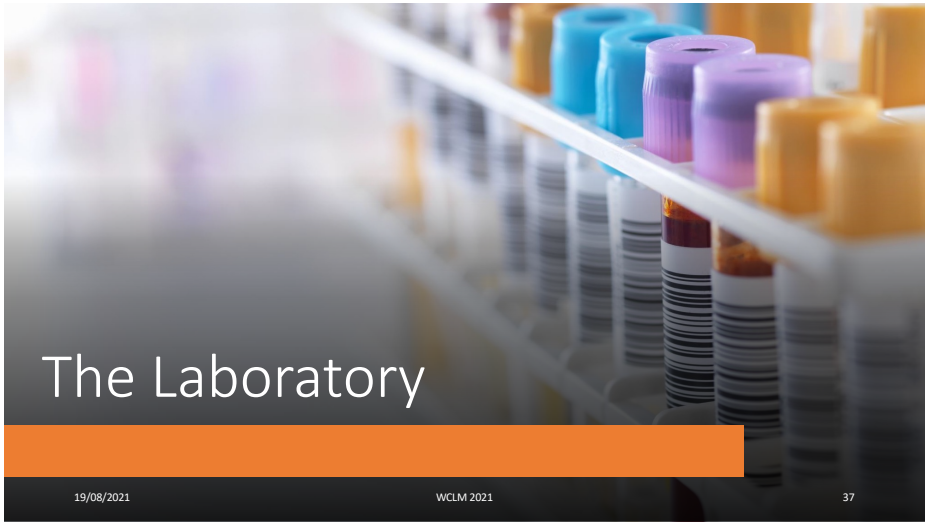
Should students give up with traditional chemistry

Can Scientific Discovery Be Automated?

Progress in the sciences can only move as fast as humans can think—outsourcing to A.I. could change that.

AHMED ALKHATEEB | APR 25, 2017 | SCIENCE

The twin challenges of too much quantity and too little quality are rooted in the finite neurological capacity of the human mind. Scientists are deriving hypotheses from a smaller and smaller fraction of our collective knowledge and consequently, more and more, asking the wrong questions, or asking ones that have already been answered. Also, human creativity seems to depend increasingly on the stochasticity of previous experiences—particular life events that allow a researcher to notice something others do not. Although chance has always been a factor in scientific discovery, it is currently playing a much larger role than it should.

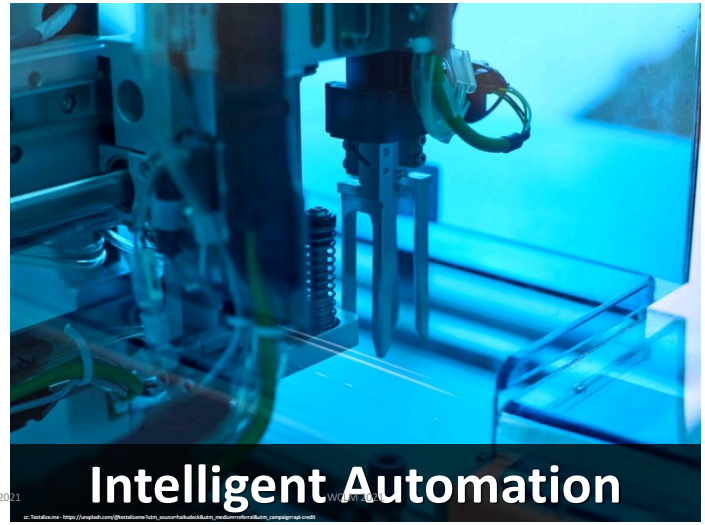


AI enabled ELNs

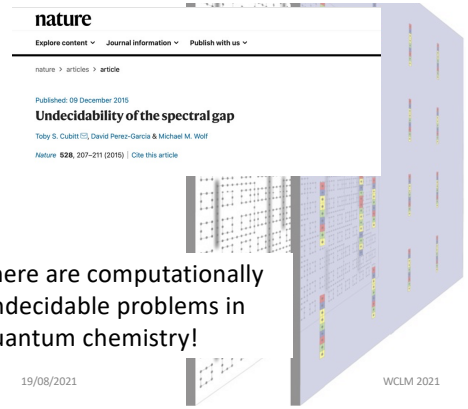
Quality annotated record
Telling the story
Machine readable

Talk2Lab

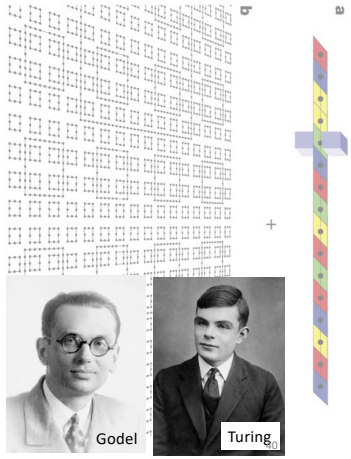
AI in the Lab

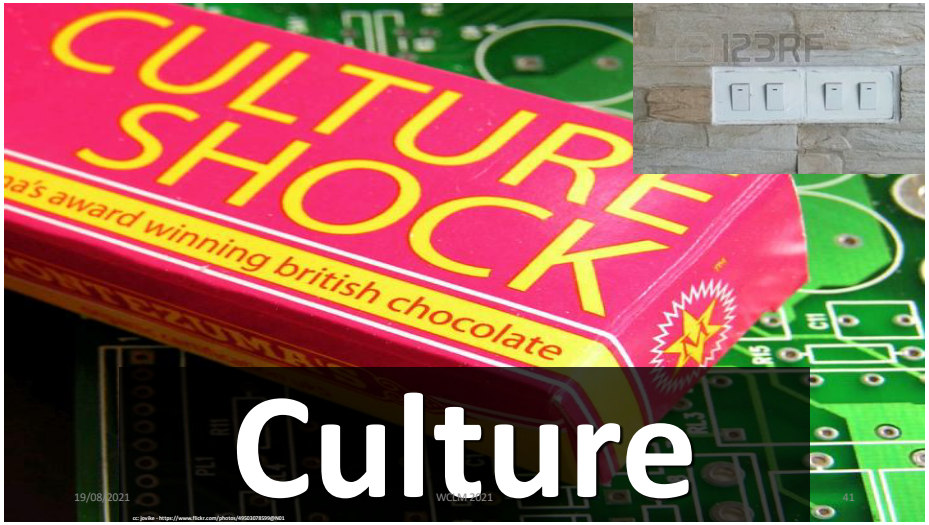


Limits of Chemical Computation



There are computationally undecidable problems in quantum chemistry!





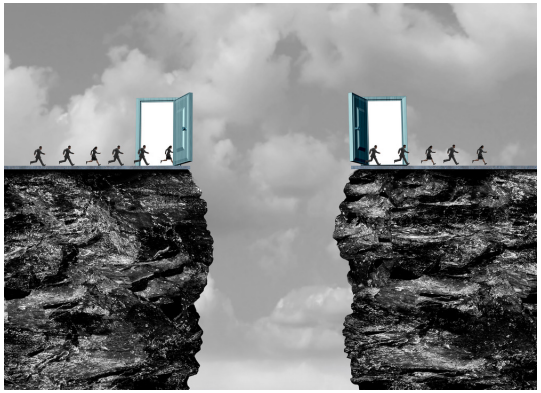
Culture

COMMUNITY

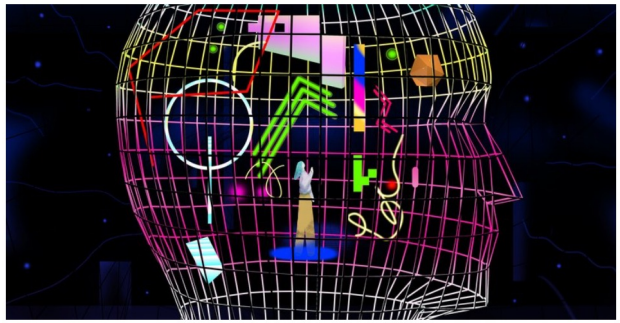
Sustainability

https://news.un.org/en/story/2015/12/519172-sustainable-development-goals-kick-start-new-year

We are still in a Liminal period



A Key worry



Overreliance on artificial intelligence may put us in intellectual debt. Illustration by Jon Han

Overreliance on AI may put us in intellectual debt

All I am saying is that now is the time to develop the technology to deflect an asteroid

Thanks

Thank you for listening

Trust me Mort - no electronic communications superhighway, no matter how vast and sophisticated, will ever replace the art of the schmooze