Professor Adham Hashibon

Institute for Materials Discovery
UCL

1. October 2025

Outline

- Lecturer: **Professor Adham Hashibon**
  - Head of the Data-Driven Materials Discovery and Informatics Group (DDMDi)
  - Module and AMS Programme lead
  - Director of the Institute for Materials Discovery
- You can contact me at: a.hashibon@ucl.ac.uk
- Moodle Page - Is being rolled over - Stay Tuned! we could review it tomorrow!
- Module Catalouge
- 4 hours every week, 3 h are lectures, and 1 h hands on tutorial.

- Lecturer: **Professor Adham Hashibon**
  - Head of the Data-Driven Materials Discovery and Informatics Group (DDMDi)
  - Module and AMS Programme lead
  - Director of the Institute for Materials Discovery
- You can contact me at: a.hashibon@ucl.ac.uk
- Moodle Page - Is being rolled over - Stay Tuned! we could review it tomorrow!
- Module Catalouge
- 4 hours every week, 3 h are lectures, and 1 h hands on tutorial.
- However, some of the lectures will be more interactive than others

Overview

What are we going to learn?

The module “Integrated Data-Driven Materials Science and Digitalisation” provides students with state-of-the art knowledge and expertise in *integrated materials* modelling, methods and practical modern advanced *cloud-based* tools to find ‘and create needed materials and process *data* for applications in advanced data-driven and *machine learning* workflows.

What are we going to learn?

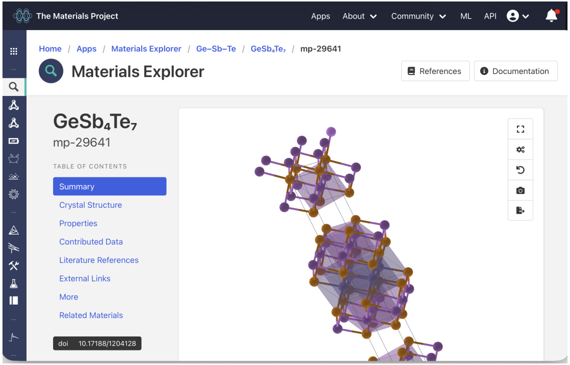
It covers contemporary topics in

- *Digitalisation* based on emerging *ontology* of materials and processes and connection to manufacturing (*digital twins*)
- *High-Throughput Computations* and *Characterisation*
- *Multiscale*, and Multi-Equation physics based modelling, including
  - Electronic density functional theory (DFT)
  - Atomistic molecular dynamics (MD)
  - Mesoscopic coarse-grained molecular dynamics (CGMD),
  - continuum structural mechanics and computational fluid mechanics (CFD) modelling,
- Enabling modelling technological applications on all relevant scales.

What are we going to learn?

Advanced modern tools include cloud-based open e-science materials digitalisation and modelling platforms such as

- nanoHUB
- Materials Project
- NOMAD Repository
- Materials Cloud — AiiDA Lab
- and other emerging platforms (like ours... name to be decided...)



Learning Objectives

- Terminology and Data Science Basics
- Gain understanding and clarity of what data-driven science means.
- Understand the roles of data-based versus physics-based modelling.
- Learn about the exciting emerging open science platforms and how to utilise them

Learning Outcomes

- Terminology and Data Science Basics
- Clear overview of the data-driven materials discovery field.
- Types of modelling.
- Bird's eye view of materials discovery.
- Understand what we want to achieve in this module and how to find additional relevant information.
- Learn about existing infrastructure and tools.

Integrated Data-Driven Materials Science and Digitalisation

- Integrated
- Data Driven
- Materials Science
- Digitalisation
- ...

Materials and Materials Science & Engineering

- Materials are almost anything we study.
- Materials Science & Engineering is about understanding the properties, processing and performance, and design of human-made materials (artefacts).

Examples

- Steels, metals, alloys
- Semiconductors
- Concrete, ceramics
- Battery materials, neuromorphic, soft matter
- Synthesis and processing, . . .
- Mechanical, thermal properties, corrosion
- Electronic structure

Human-Made Materials vs. Life on Earth

- Human-made materials now equal the weight of all life on Earth.
- Rapid growth in concrete, asphalt, metal, and plastic.
- 2020 may mark the tipping point where artificial materials outweigh living things.
- Study highlights the literal massiveness of humanity's planetary footprint.

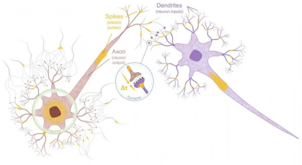
Sources: Scientific American, *Human-Made Stuff Now Outweighs All Life on Earth*, scientificamerican.com

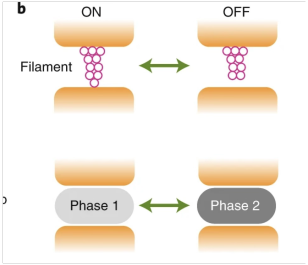
National Geographic, *Human-made materials now equal weight of all life on Earth*,

nationalgeographic.com

Did You Know

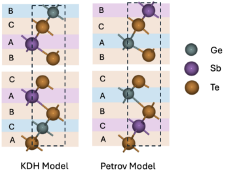
- Neuromorphic computing is inspired by the structure and function of the human brain.
- Schematics show memristive switching by filament formation and rupture (top) or phase change (bottom).
- The way the filament changes phase in response to stimuli could offer a pathway for ”learning”.
- This behavior is comparable to the axon in a biological neuron.
- The Intel Loihi uses neuromorphic computing principles, yet relies on traditional metal-oxide semiconductors.

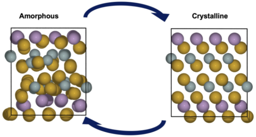


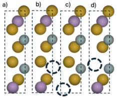


Neuromorphic Materials: Chalcogenides

- **Chalcogenides** are a class of phase-change materials (PCMs)
- Can reversibly switch between an *amorphous (glassy)* phase and a *crystalline* phase, triggered by thermal energy or electric fields.
- This switching enables **non-volatile memory** (e.g., PC-RAM), which retains data without power.
- **Computational materials modelling** helps study their atomistic and electronic behavior:
  - Phase transitions and energy barriers
  - Thermodynamic stability and mechanical properties
  - Thermal and electronic transport

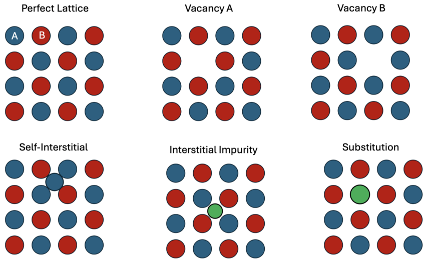






Point Defects in Crystals

- Crystals are not perfect, they contain various types of defects!
- The simplest defects are **Point defects**:
  - **Vacancies**: Missing atoms
  - **Self-interstitials**: Extra atoms squeezed into the lattice
  - **Interstitial impurities**: Foreign atoms occupying spaces between lattice sites
  - **Substitutional impurities**: Foreign atoms replacing host atoms
- These defects affect electronic transport, thermal conductivity, and phase stability

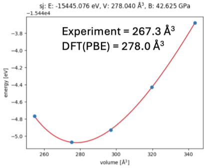


Example of DFT calculation

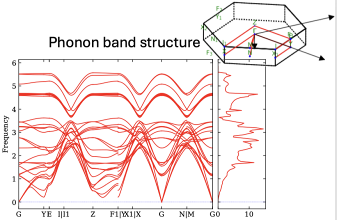
Neuromorphic Materials

- Quantum mechanical methods (e.g. DFT) allows us to calculate the properties of materials from first principles
- Calculate electronic and vibrational properties (band structure, DOS, band gaps, defect energies)

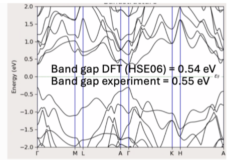
Birch-Murnaghan



Phonon band structure

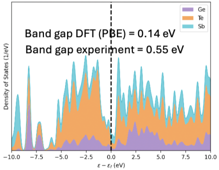


Band structure

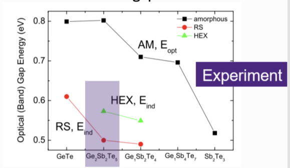


Improved method

Electronic DOS



Band gap



**J. W. Park, S. H. Eom, and H. Lee, Phys. Rev. B 80, 115209 (2009).

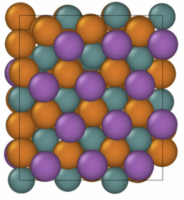
Example of MD calculation

Neuromorphic Materials

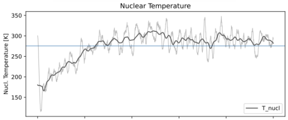
- Molecular dynamics simulations allows us to study as $Ge_2Sb_2Te_5$ as a function of time through solving Newton's equations of motion
- Simulate the materials and account for temperature
- Gain insights missed with static calculations (*e.g*. lattice dynamics, transport phenomena)
- Use different level of theories, *ab initio* (quantum mechanics) or force fields (classical mechanics)

$$\overline{F} = -\nabla E = m\overline{\frac{dv}{dt}} = m\overline{\frac{d^2x}{dt^2}}$$

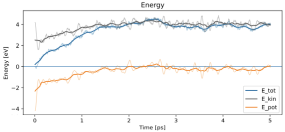
Ongoing work by O. Beynon (UCL IMD/DDMD group)



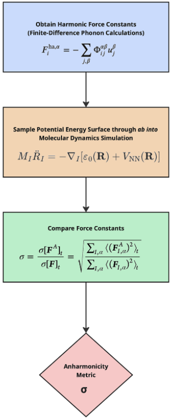
Simulation at RT (300K) →

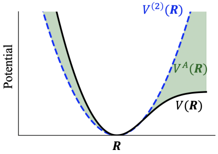


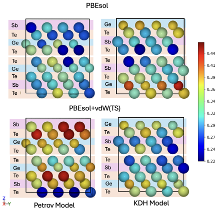
Ab initio MD using DFT (GGA XC functional)



Neuromorphic Materials Layout







- Anharmonic effects are important!
- (Owain, Hashibon, in preparation, 2025)

Data-Driven Materials Science

Leverage data to extract knowledge, rather than relying mainly on traditional theory or physics-based modelsi or empirical knowledge.

- Data becomes a key driver of discovery and innovation.
- This approach contrasts with classical methods rooted in mathematics and physical theory.
- The shift: *From equations to correlations, from models to patterns*.
- *Data is not just a result any more but it is the* **engine of knowledge**
- But we still and in addition, look at materials modelling, where simulations and computational methods generate valuable data.

The role of Digitalisation in Data-Driven Materials Science

- **Data-Driven Systems** shift the paradigm from theory-based to information-based discovery.
- **Materials Modelling** generates data that fuels knowledge extraction.
- This approach supports the concept of a **Digital Twin**—a virtual replica of a material or process.
- We move from physical experimentation to *computational exploration*.

Digitalisation of materials enables us to process and understand materials without direct physical interaction, working instead with their digital representations –¿ Digital Models.
Digitalisation is not just a tool—it's a transformation of how we do materials science.

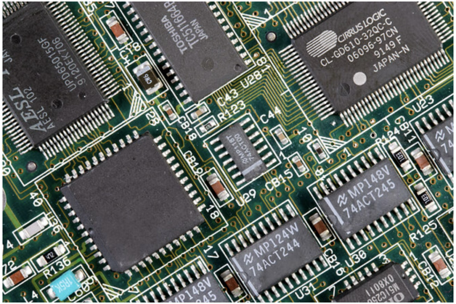
Digitalisation

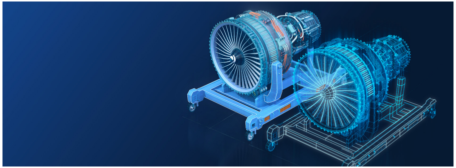
Dictionary definition:**digitalization** — (digitalisation)
noun [mass noun]
adaptation of a system, process, etc. to be operated with the use of computers and the internet:
digitalization allowed companies to sell goods without a physical presence

to Process "material" without their physical presence = working with the information about the material.

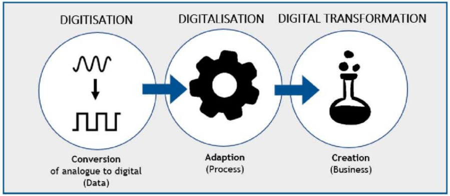
This is the so called **Digital Twin**

image credit: 3ds





Digitalisation vs Digitisation

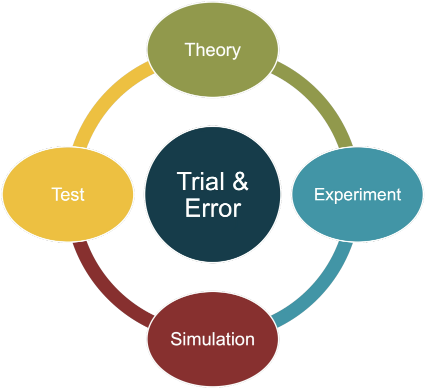


Buman and Mark

- **Digitisation**: Conversion of physical formats (e.g., paper, stone) into digital media (e.g., disk, memory).
- **Digitalisation**: Goes beyond digitisationr, it's about transforming processes and systems using digital technologies
- Raises the question: *What does digitalisation mean for materials science?*

Traditional Materials Discovery

- Use experiments and empirical knowledge to suggest materials or optimise existing ones
- Focuses on a particular material, and sometimes also a process (though often neglected)
- Example: *"What are the mechanisms of Li conductance in M_3N ($M = Nb, Ta$)?"*
- Test and repeat: Generate small, targeted number of experiments and simulations
- (Very) Small amount of data

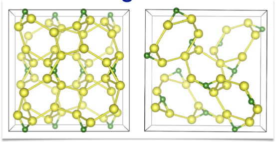


A Typical Example...

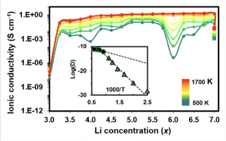
Traditional paradigm leads to success …but is time consuming

~ 4 years turnaround

- Assume 50 (materials) x 10 (processes) x 10 (parameters) = 5000 different options in the design space for Li ion batteries.
- Each study (trial) requires, optimistically, 1 PhD (3 years)
- 15000 years of development time (total).
- How many PhDs are there per year? …. say 1000!
- Then we get 15 years on average for developing new materials and process to produce new batteries.



Li sublattice in Garnet electrolytes for two Li concentrations (x =7 (left), x =6



Ionic conductivity (S/m) of Li^+

Kozinsky et. Al. (2016). Effects of Sublattice Symmetry and Frustration on Ionic Transport in Garnet Solid Electrolytes. *PRL*, *116*(5). https://doi.org/ARTN 05590110.1103/PhysRevLett.116.055901

The actual history of Li-ion battery

P. M. Pancorbo, *Cradle-to-Gate Life-Cycle Assessment of Future Materials for Commercial Lithium-Ion Batteries: Raw Materials Issues*, (2018).

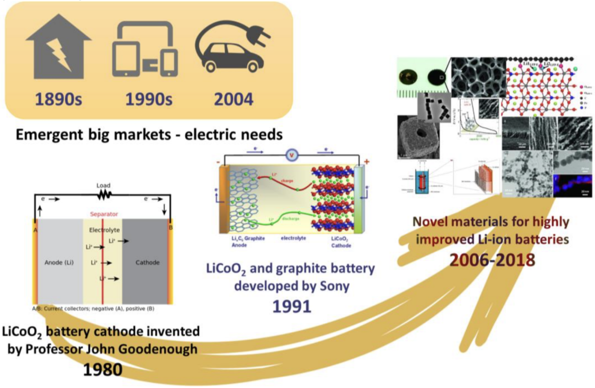
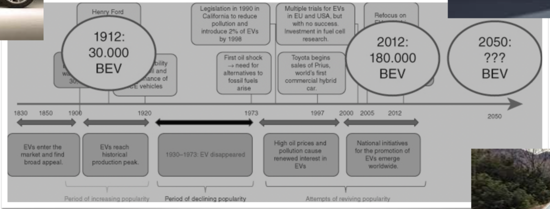


Figure 1. Diagram of the historical development of Li-ion batteries to address the electric needs (mix of images from different sources [7]–[11])

Did you know that...

Institute for Materials Discovery (IMD)



WE really went in the wring direction!

Why? (Hint: business first!)

More about this sort of interesting things is in NSI0021

NSCI0032 - (C) Prof A. Hashibon - UCL - Term 1 2023 34

Self-Starting Cadillac, 1912

From *Toronto Sunday World*, Feb. 18, 1912.
The release of the first practical electric self-starter on the 1912 Cadillacs was a major event.
Contemporary reports said that the new technology was "of more interest to motorists than any other."
The self-starter also established the need for electrical systems on future gasoline cars, creating a much more lucrative industry for battery companies than for powering electrics.