

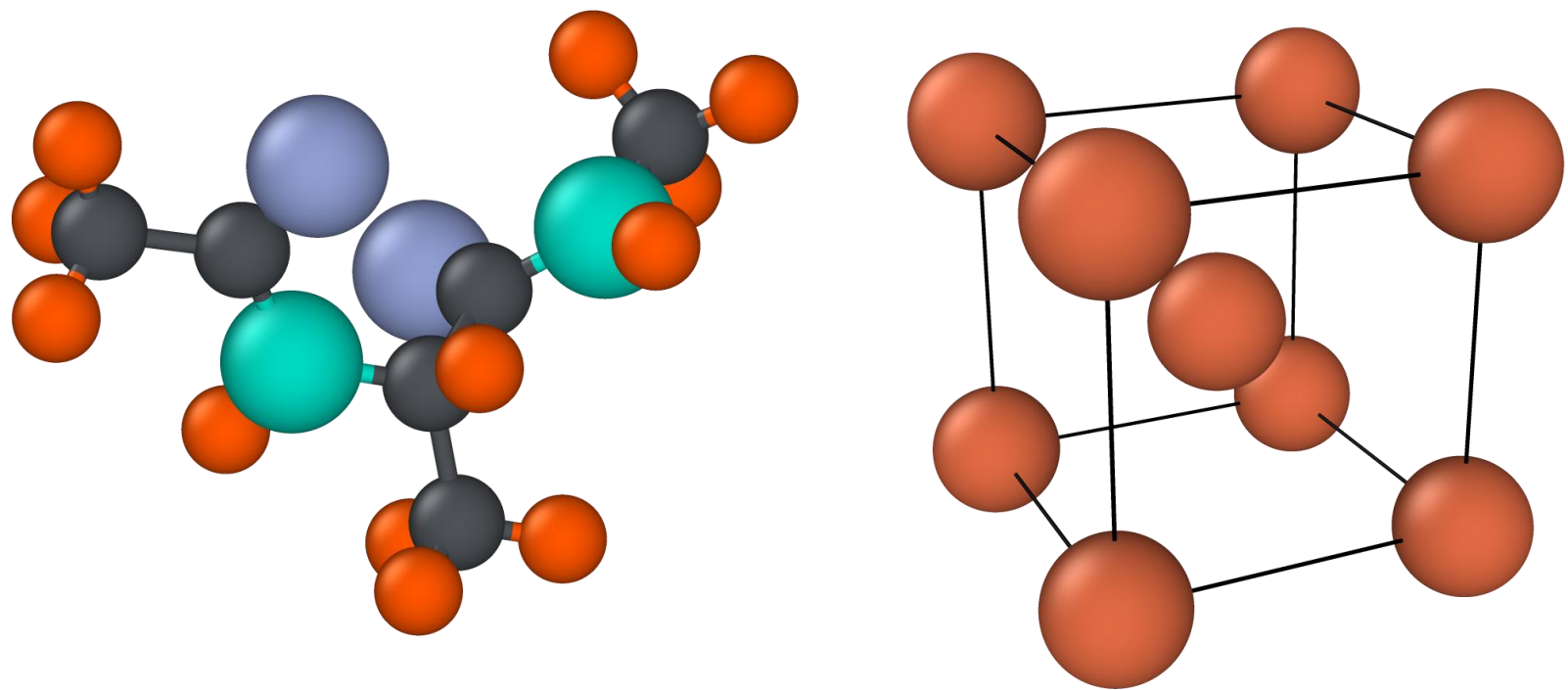


Machine Learning the Interactions Between Atoms

Fraser Birks, James Kermode

Why Simulate Atoms?

To make predictions about **molecules** and **materials**



Active research areas

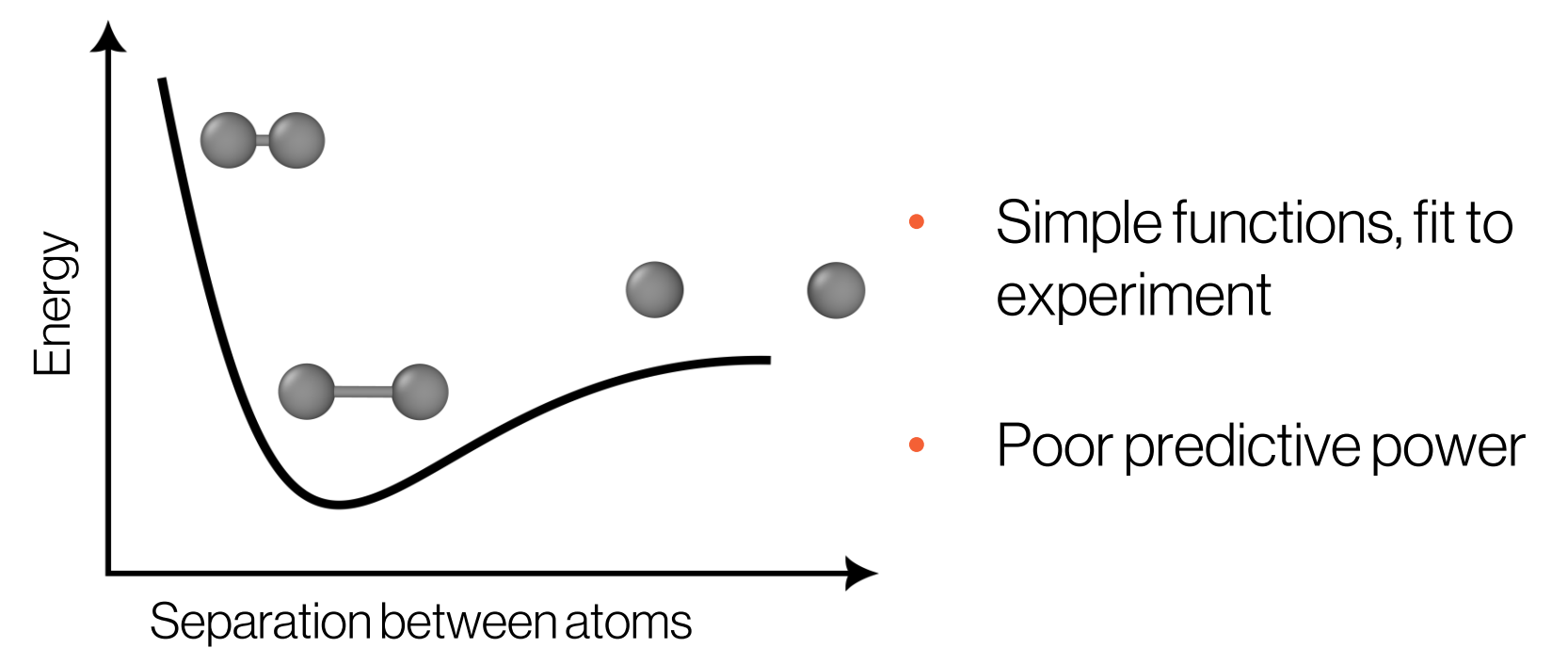
- Drug discovery
- Catalysis
- Batteries
- Nuclear power

Engaged companies

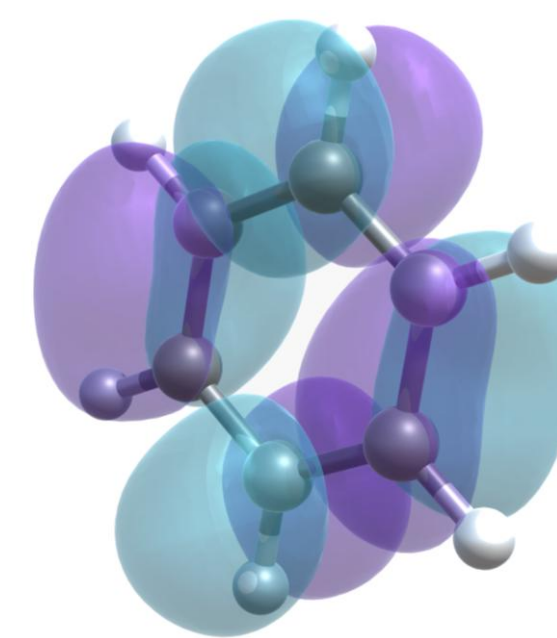
- Meta
- Microsoft
- Google
- NVIDIA

Conventional Methods

Empirical models – **fast** but **inaccurate**



Quantum mechanics – **accurate** but **slow**

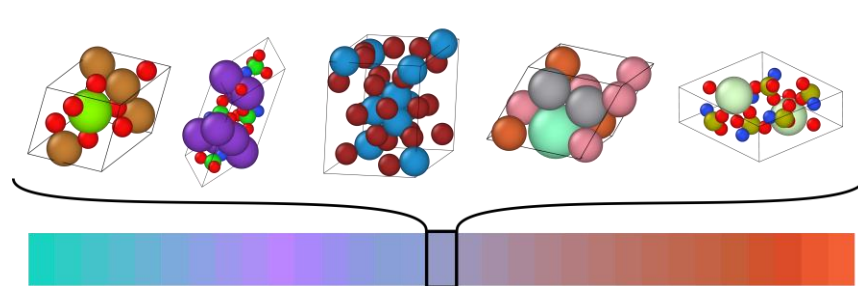


- Electron interactions simulated directly
- Limited to **a few hundred atoms** for a **few picoseconds** (trillionths of a second)

Machine Learning

Aim: to simulate atoms at **quantum mechanical accuracy**, but **millions of times faster**

- Step 1: Build dataset

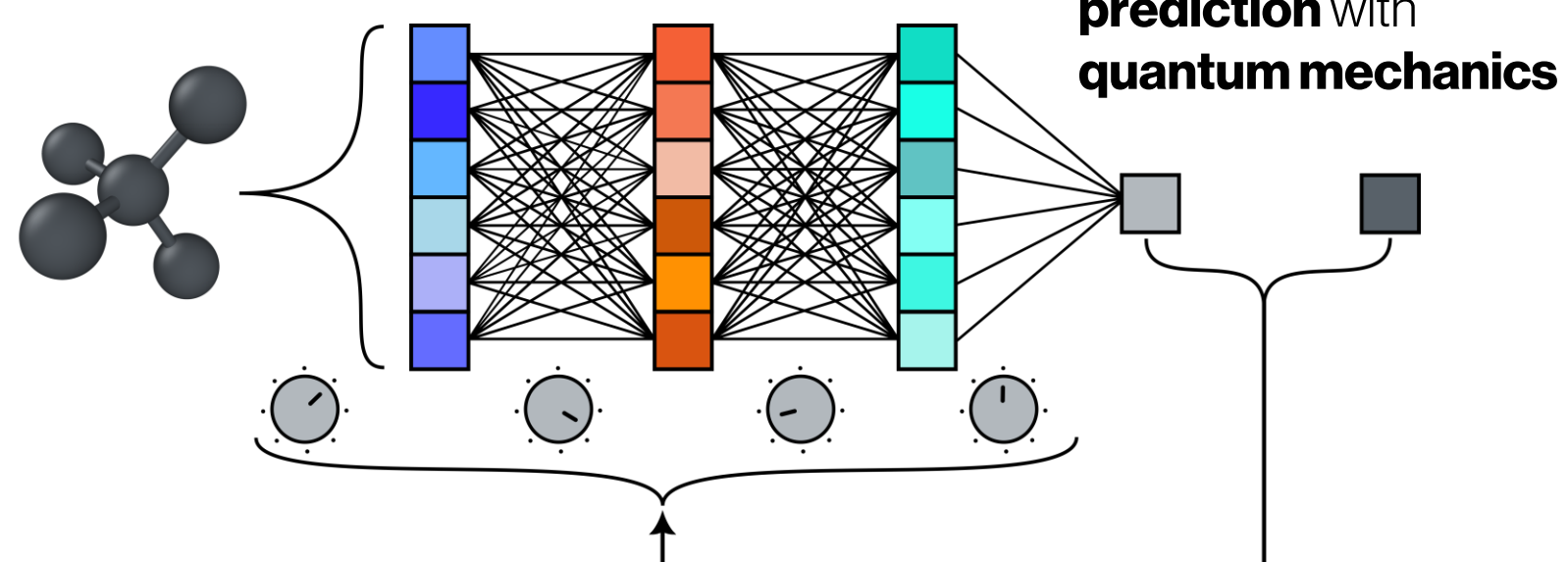


Each structure analysed using **quantum mechanics**

Large dataset – millions of small structures

- Step 2: Train model

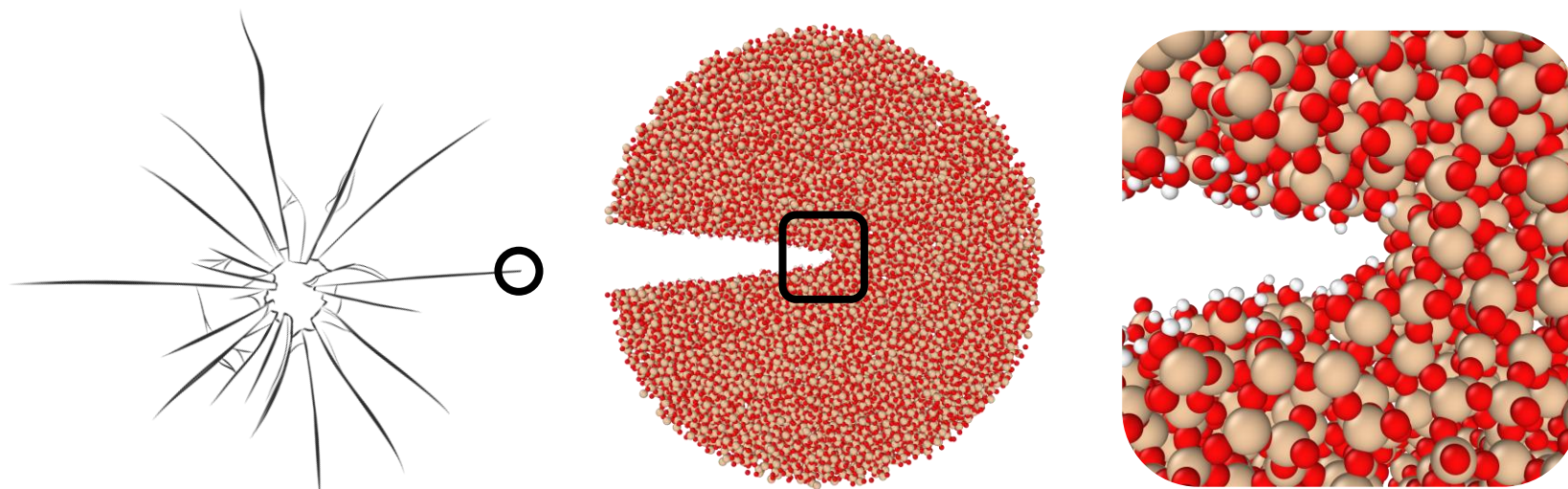
1. Feed **each structure** into model



2. Compare **prediction** with **quantum mechanics**

3. Adjust **model parameters** to improve prediction

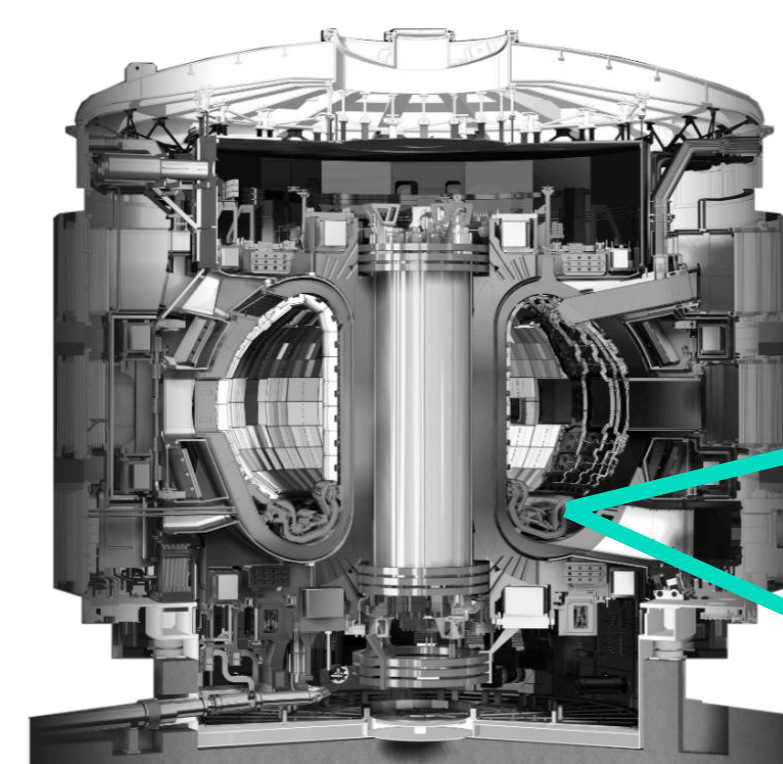
- Step 3: Simulate **large structures for long timescales**



Simulation of **crack growth** in **window glass**

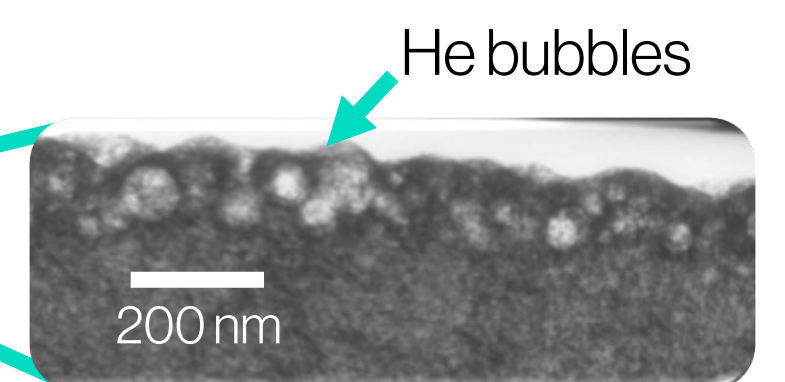
Application: Nuclear Fusion

Controlled nuclear fusion could provide **limitless clean energy**.



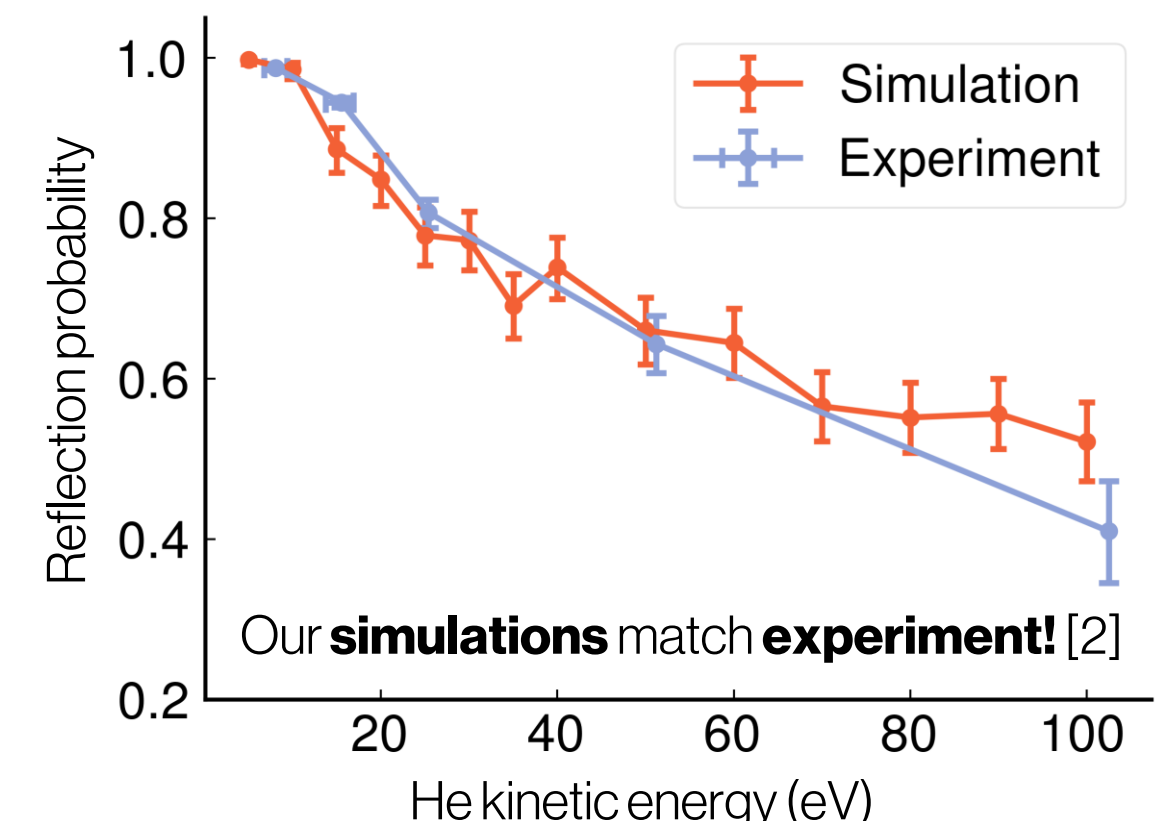
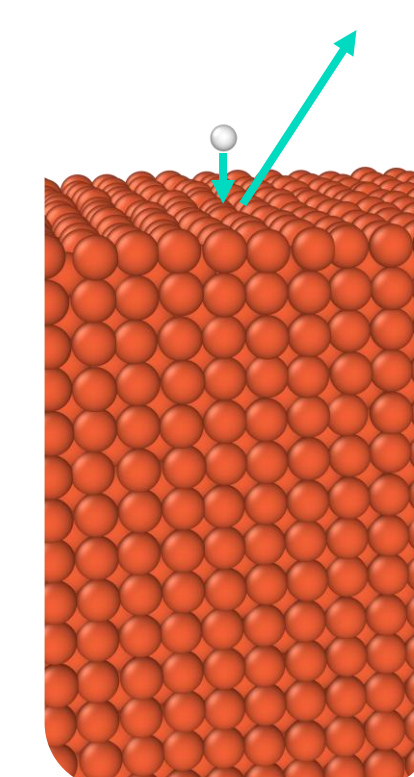
Tokamak fusion reactor, ITER

Problem: helium bubble formation on internal surfaces



Plasma-facing tungsten surface [1]

We use **simulations** to predict the **probability** of **impacting helium** entering the **plasma-facing tungsten surface**



[1] Kajita et al., Phys. Scr. 89, 025602 (2014).

[2] van Gorkum & Kornelsen, Radiation Effects 52, 25–33 (1980)