Fighting Climate Change with Quantum Mechanics

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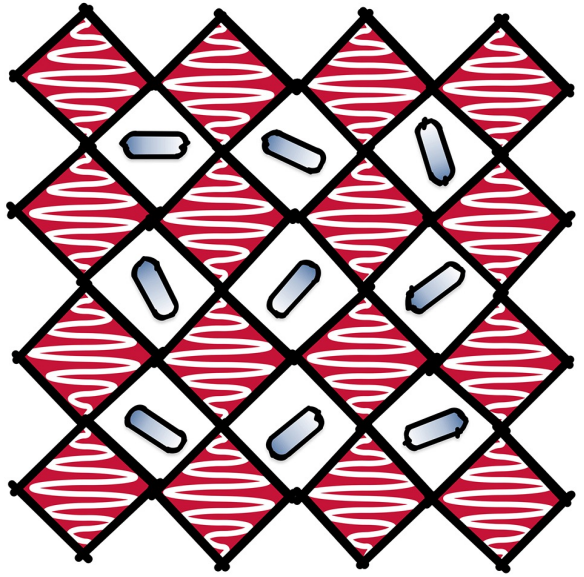
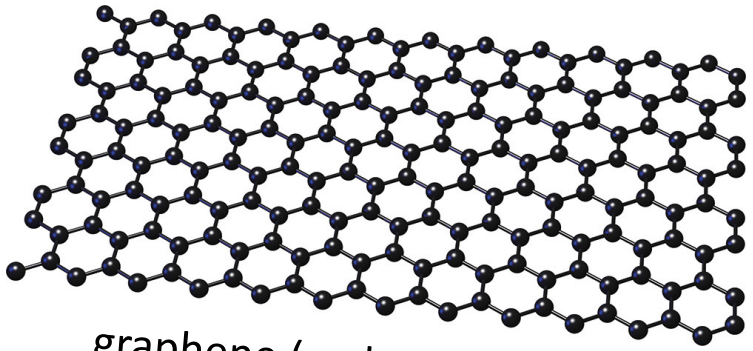
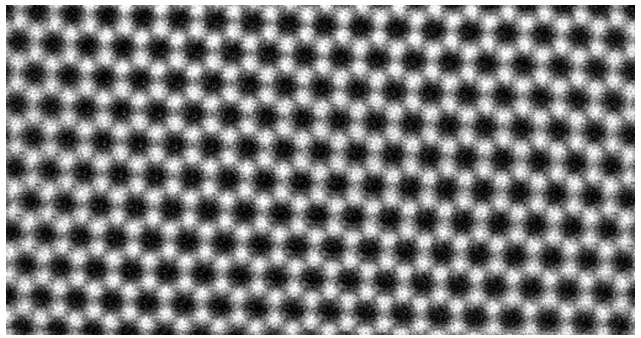


Schrödinger equation

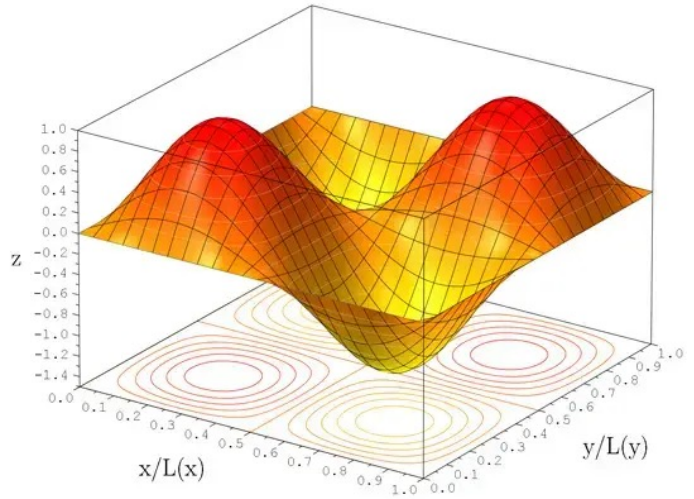
$$\hat{H}\Psi = E\Psi$$

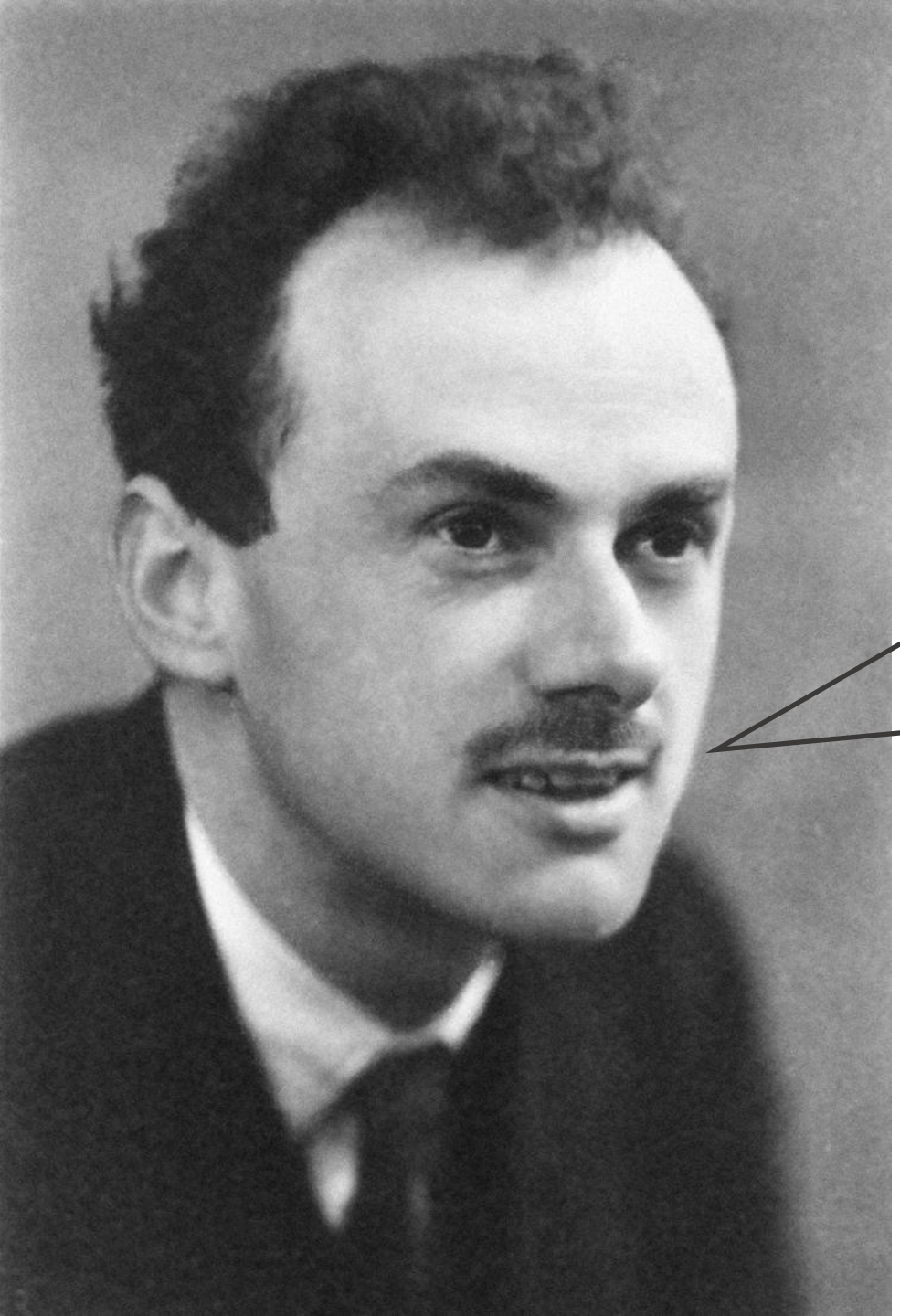


graphene (carbon)



electron microscope image

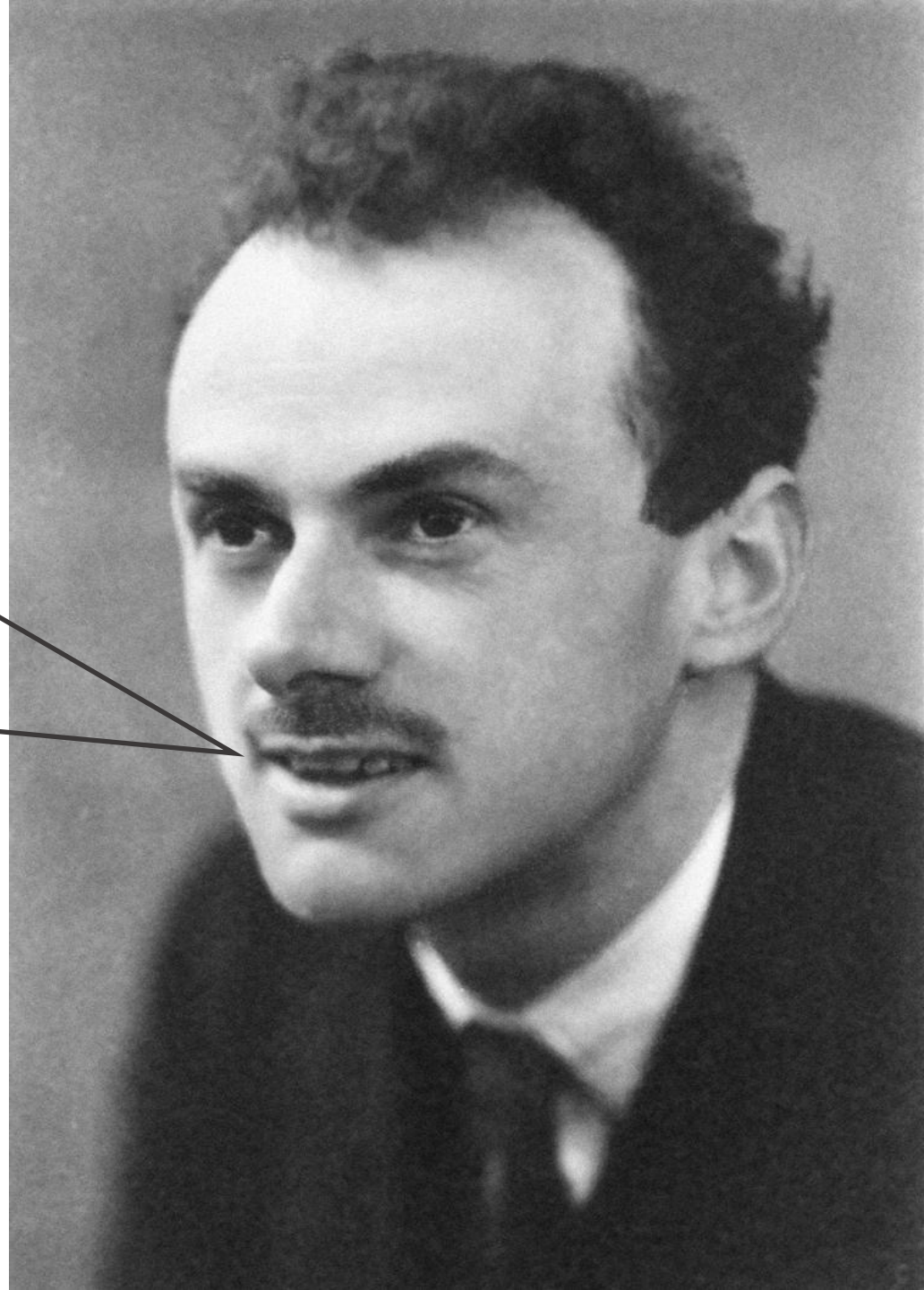




The underlying physical laws necessary for a large part of physics and the whole of chemistry are thus completely known...

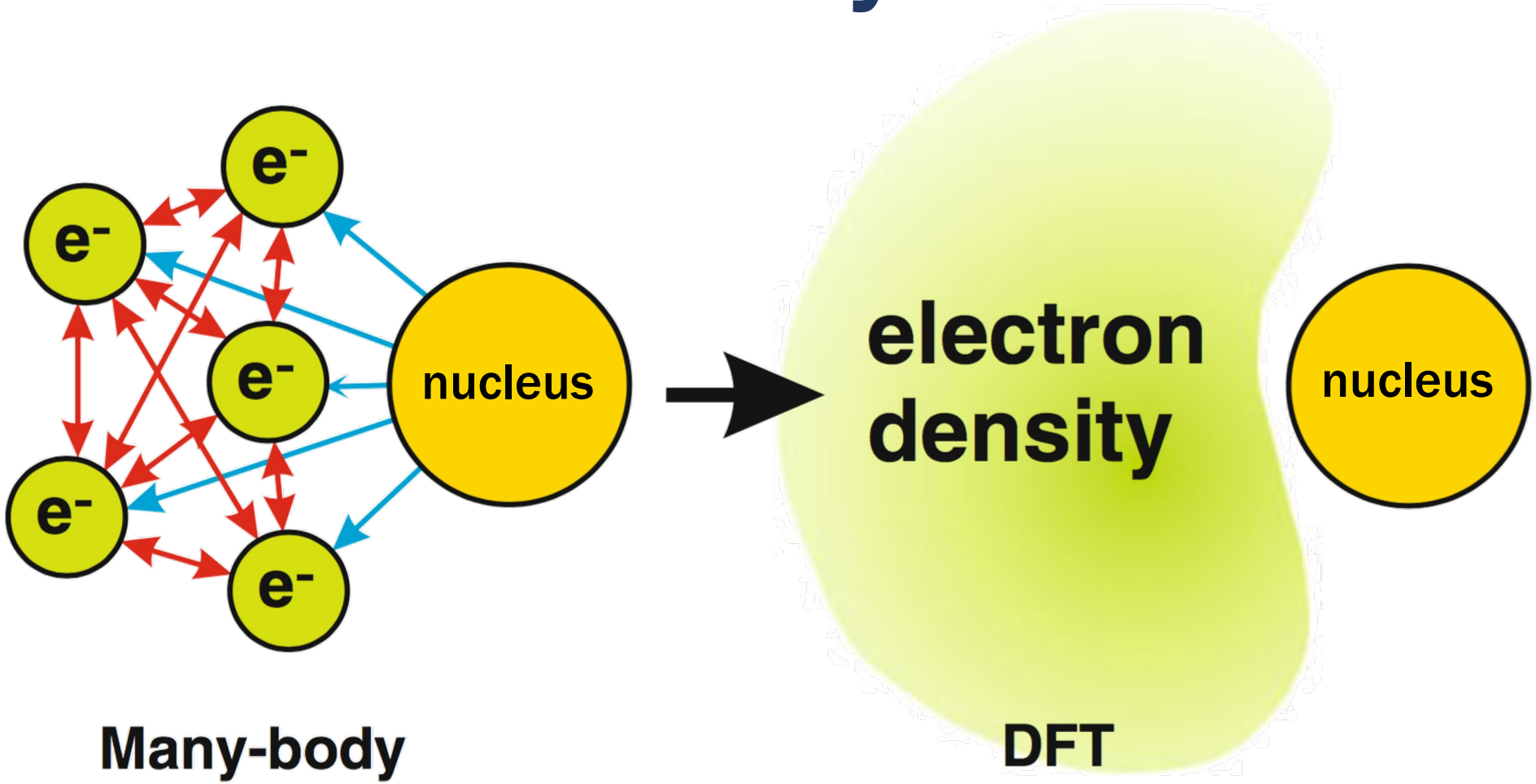
Quantum mechanics of many-electron systems
Paul Dirac, 1929

....and the difficulty is only that the exact applications of these laws lead to equations much too complicated to be soluble.



Quantum mechanics of many-electron systems
Paul Dirac, 1929

Quantum chemistry to the rescue!



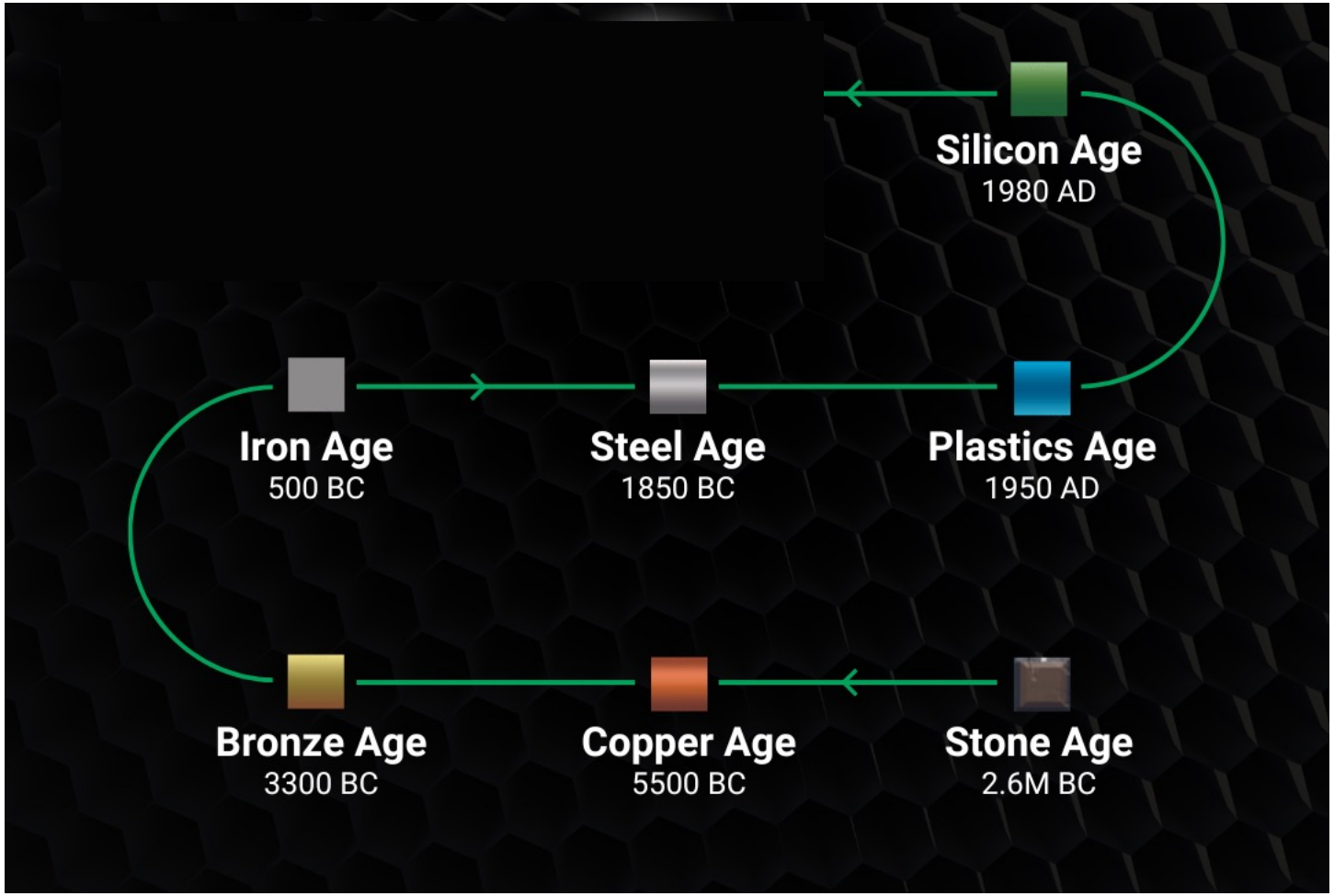
Exascale (10^{18}) supercomputing

Installation of the UK Supercomputer “Archer2”

System	Cores	Rmax (PFlop/s)
Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,194.00
Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01
LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,220,288	309.10
Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, Atos EuroHPC/CINECA Italy	1,824,768	238.70

Top500.org

Every major advance in human civilization has been driven by Materials Science



See: *Fundamental Materials Research and the Course of Human Civilization*
Prof. Nicola Spaldin

We are now in the era of anthropogenic climate change

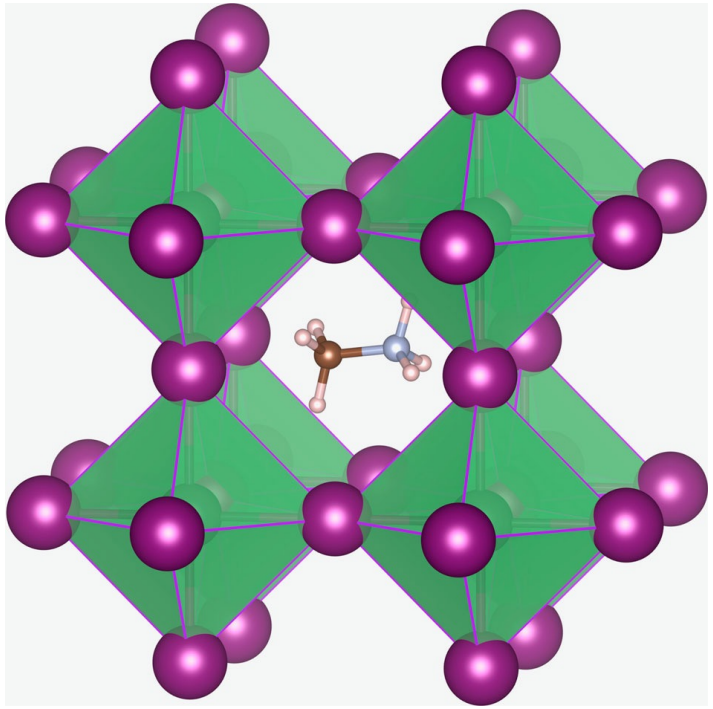
We need new materials for energy conversion and storage

More efficient solar cell (photovoltaic) absorbers

Lighter wind-turbine blades

Energy dense rechargeable battery cathodes

Perovskite: the next super-material?



$CaTiO_3$

inorganic

1839

$CH_3NH_3PbI_3$

hybrid

2009

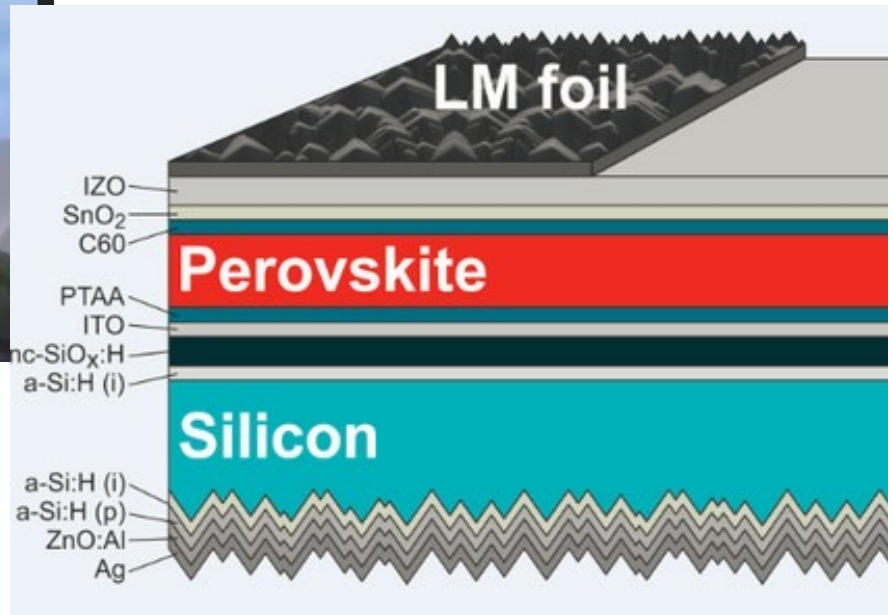
Perovskite: a record-breaking material

Tech

‘Miracle material’ smashes solar panel efficiency threshold

Breakthrough paves way for mass-production of ultra-efficient perovskite solar cells

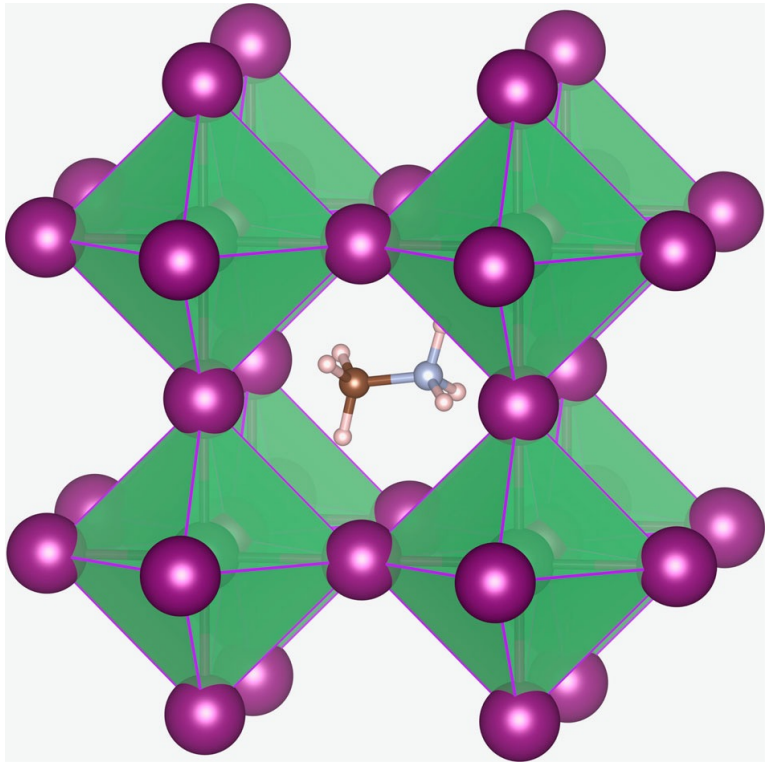
Anthony Cuthbertson • Sunday 09 July 2023 08:57 BST • 3 Comments

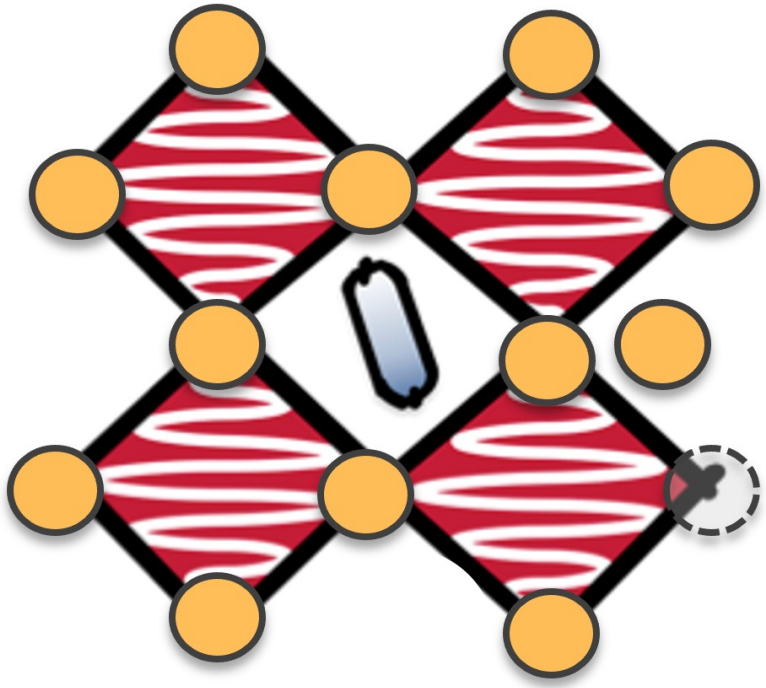


Silicon only → Perovskite on silicon

29% → 33%

Perovskite: a mysterious material

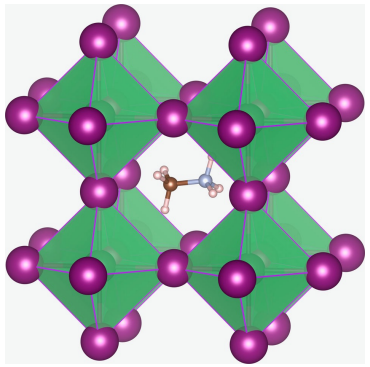


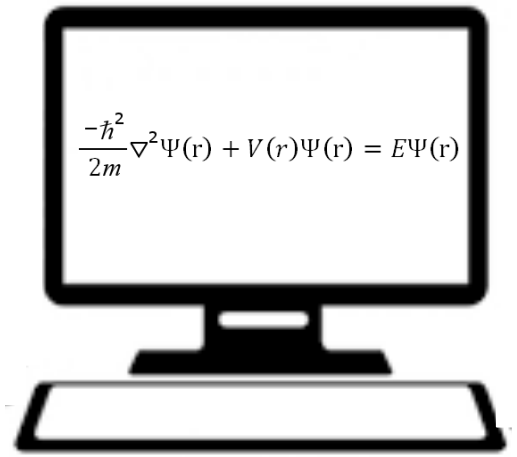


$CH_3NH_3PbI_3$

<u>Defect-tolerant</u>: defects do not kill solar cell performance

Materials design accelerated with computers





Band gap

Bulk modulus

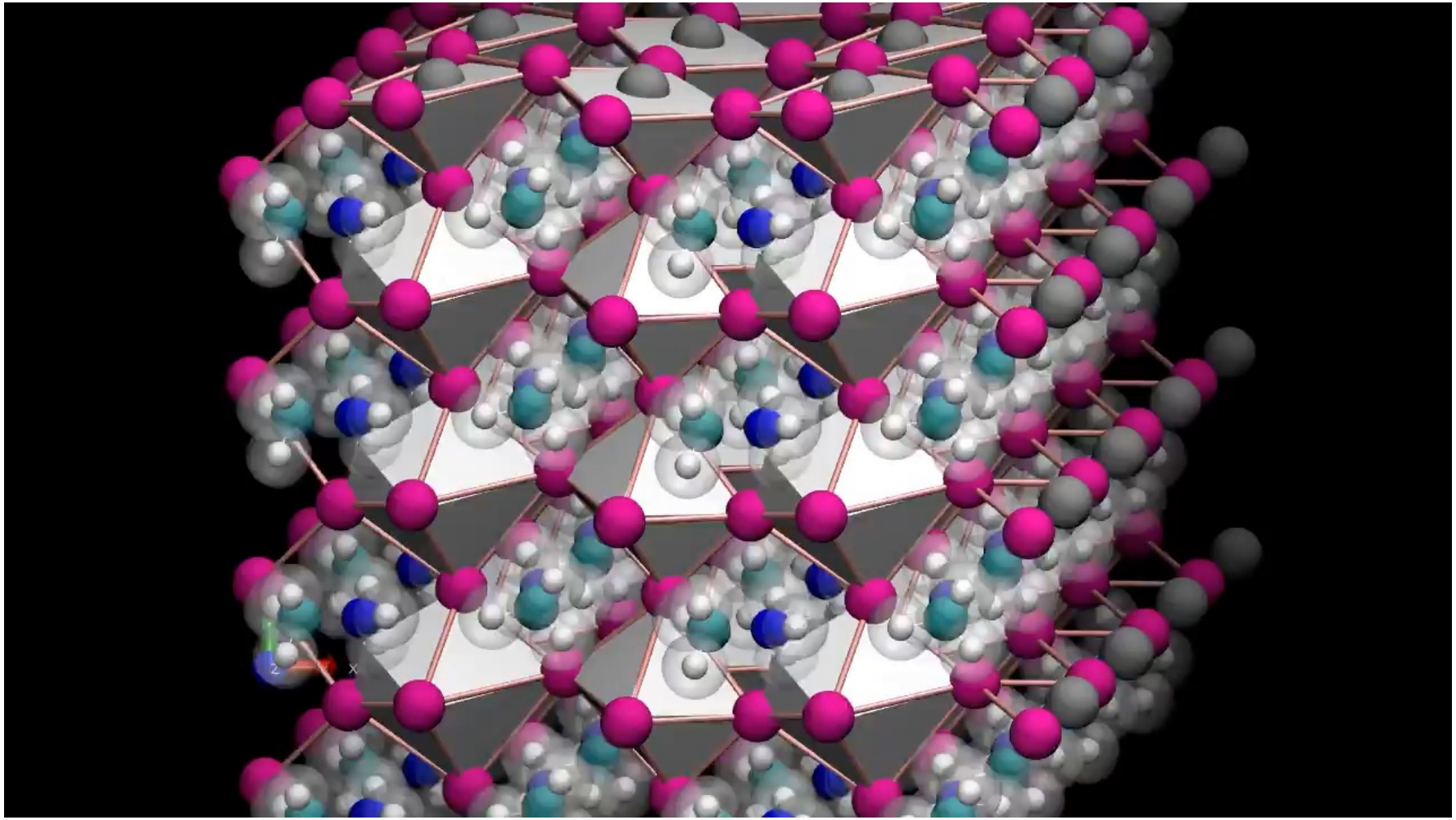
Electrical conductivity

Curie temperature

Thermal expansion

Input composition and structure → **Solve Schrödinger Equation** → **Output properties**

Predicting atomic scale vibrations



Courtsey Dr Jarvist Frost

Latest research! large distortions → defect tolerance

Our latest research* shows that large atomic-scale distortions de-activate “killer” defects

stiff material

flexible perovskite material

electron

* *Journal of Physical Chemistry C* 2023, 127, 32, 15738–15746

Thanks for listening

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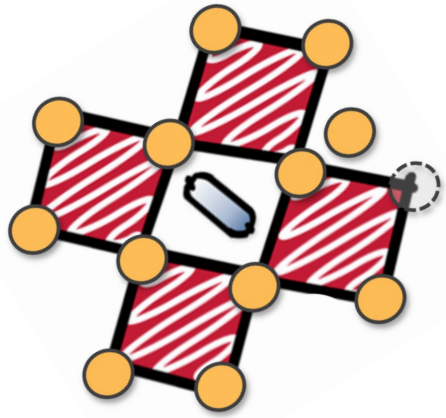
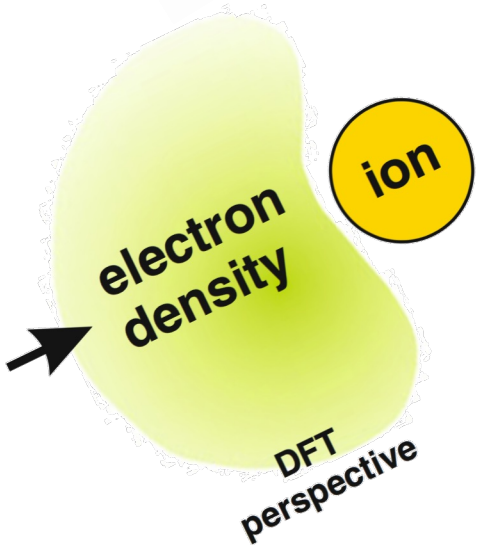
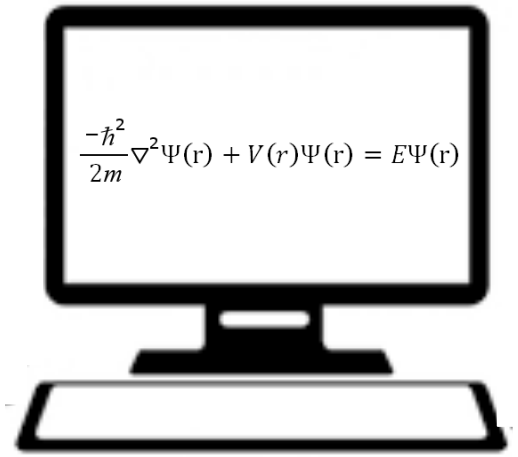
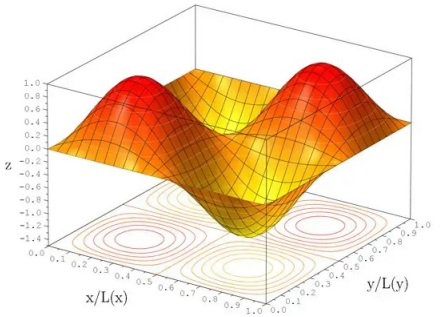
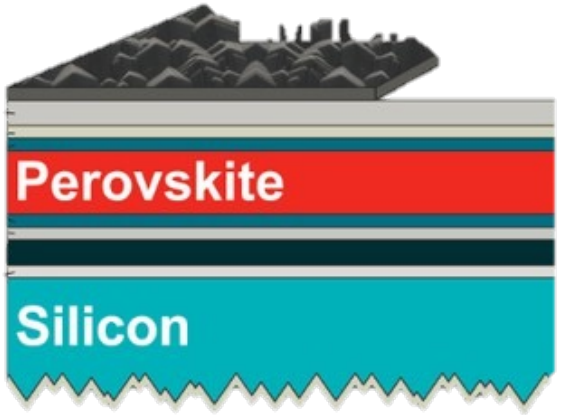






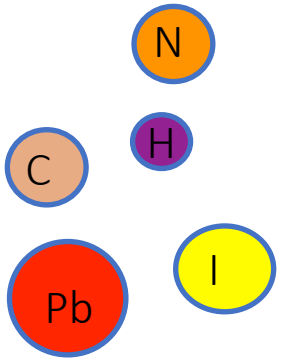




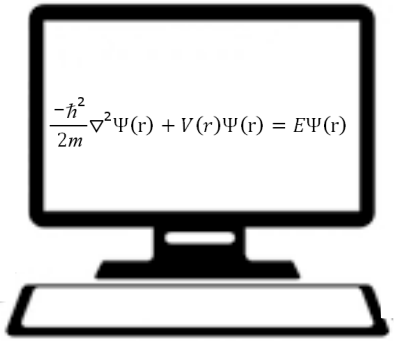
Perovskite production line, Brandenburg an der Havel (Germany)

oxfordpv.com

Materials design accelerated with computers

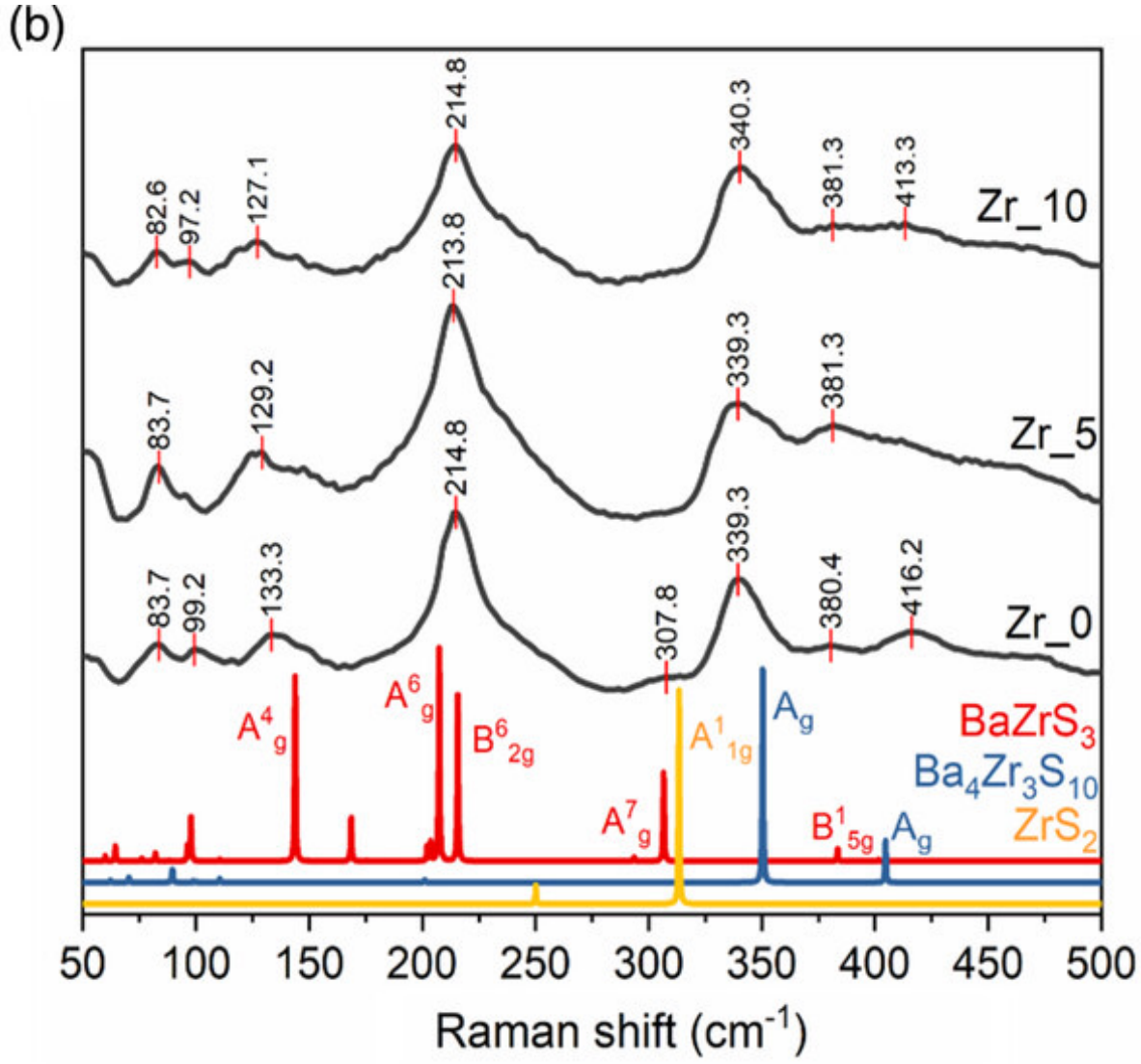


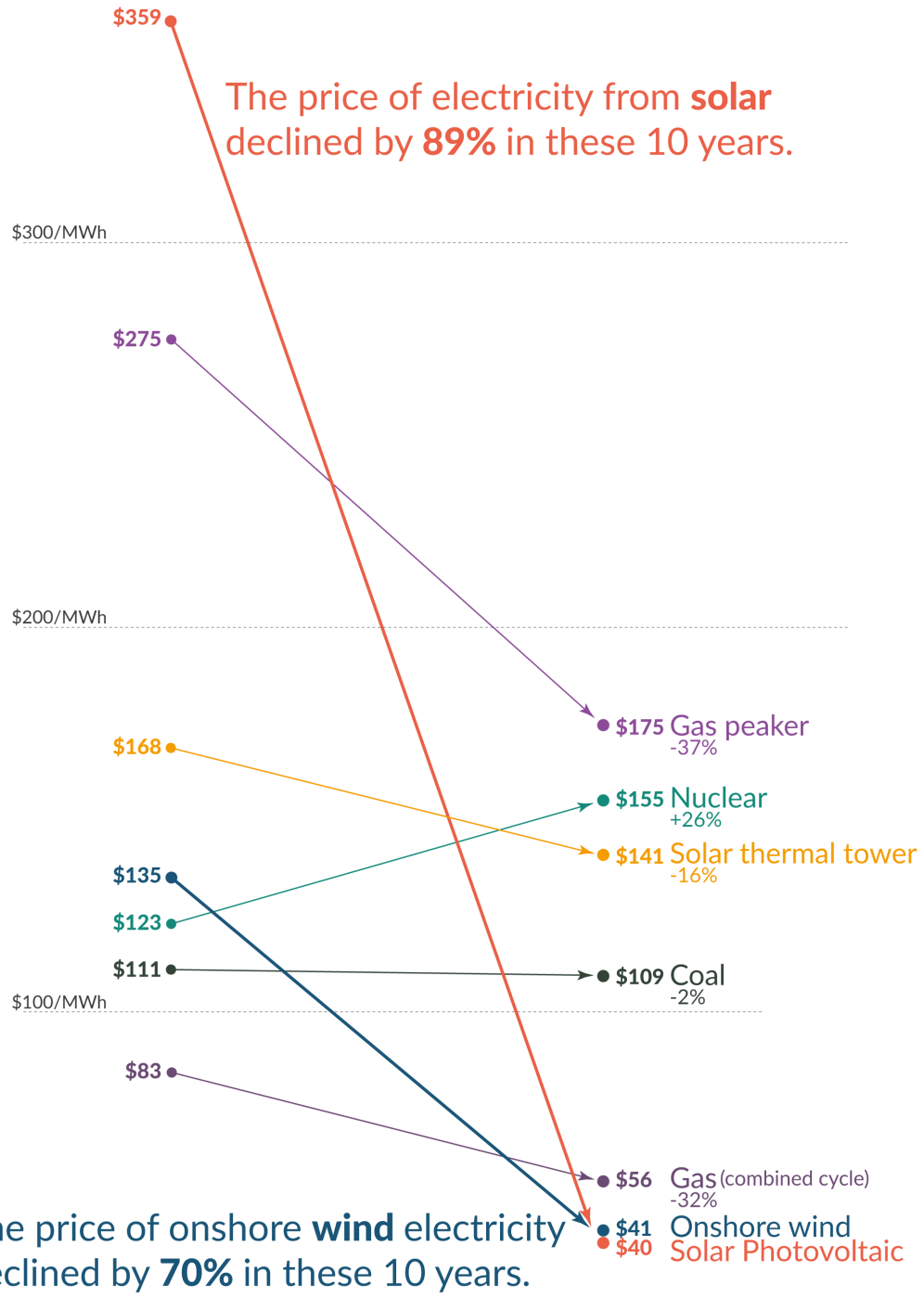
Input Composition



Solve Schrödinger Equation

We can predict the unique vibrational fingerprints of materials for comparison against experiment





Success comes with a caveat

See: *The co-evolution of technological promises, modelling, policies and climate change targets*
McLaren and Markusson