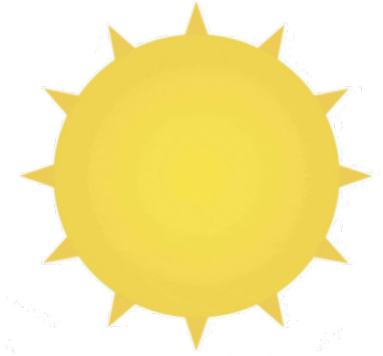


Fighting Climate Change with Quantum Mechanics

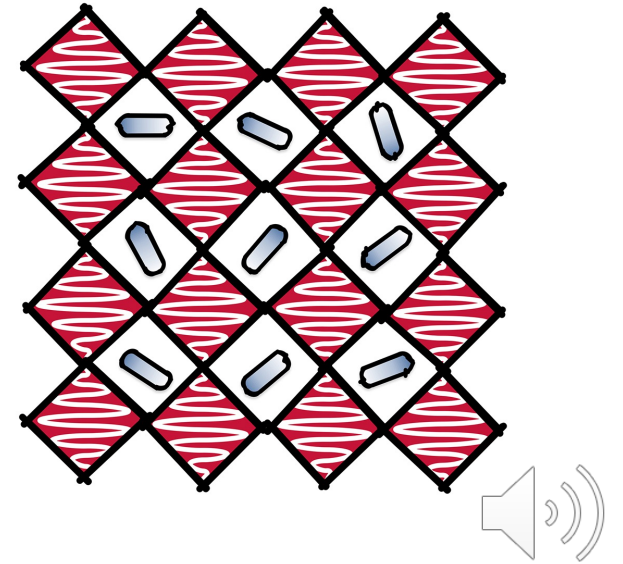


Dr Lucy Whalley

Assistant Professor in Physics
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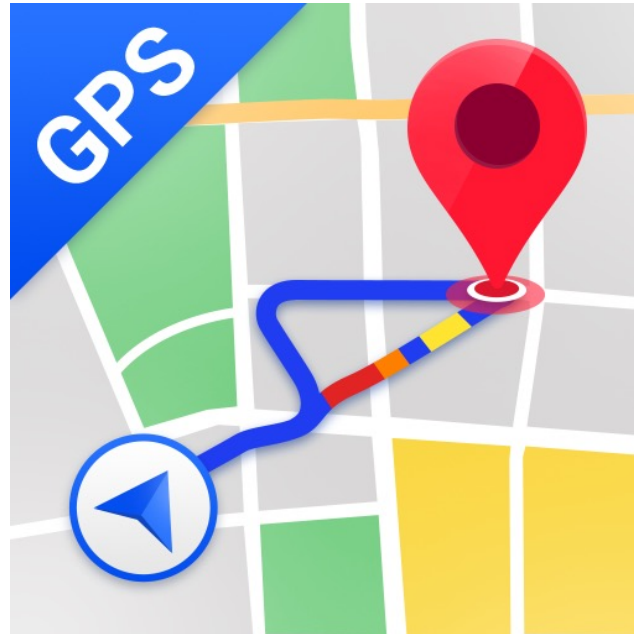
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Website: lucydot.github.io

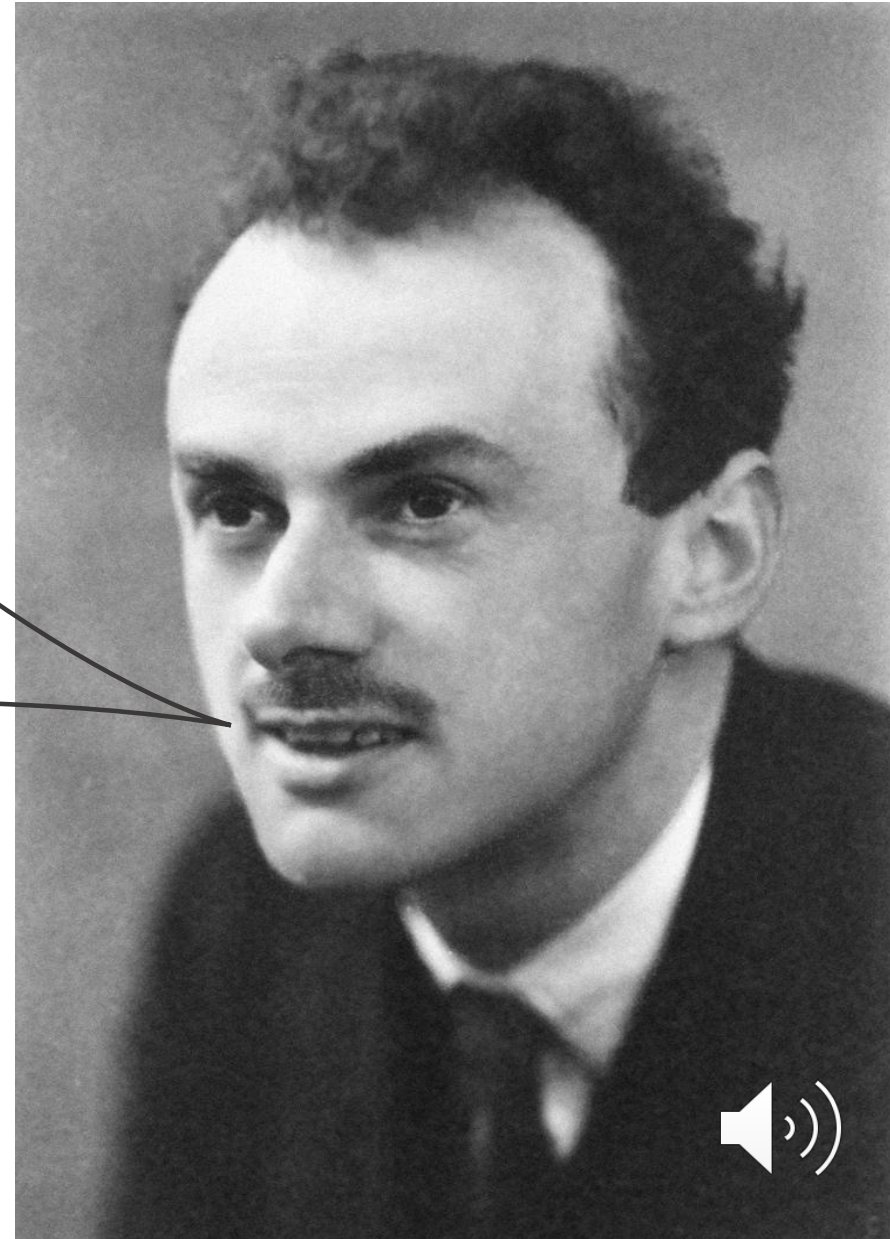


Schrödinger equation [1925]

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



.... the exact applications
of these [quantum
mechanical] laws lead to
equations much too
complicated to be
soluble.

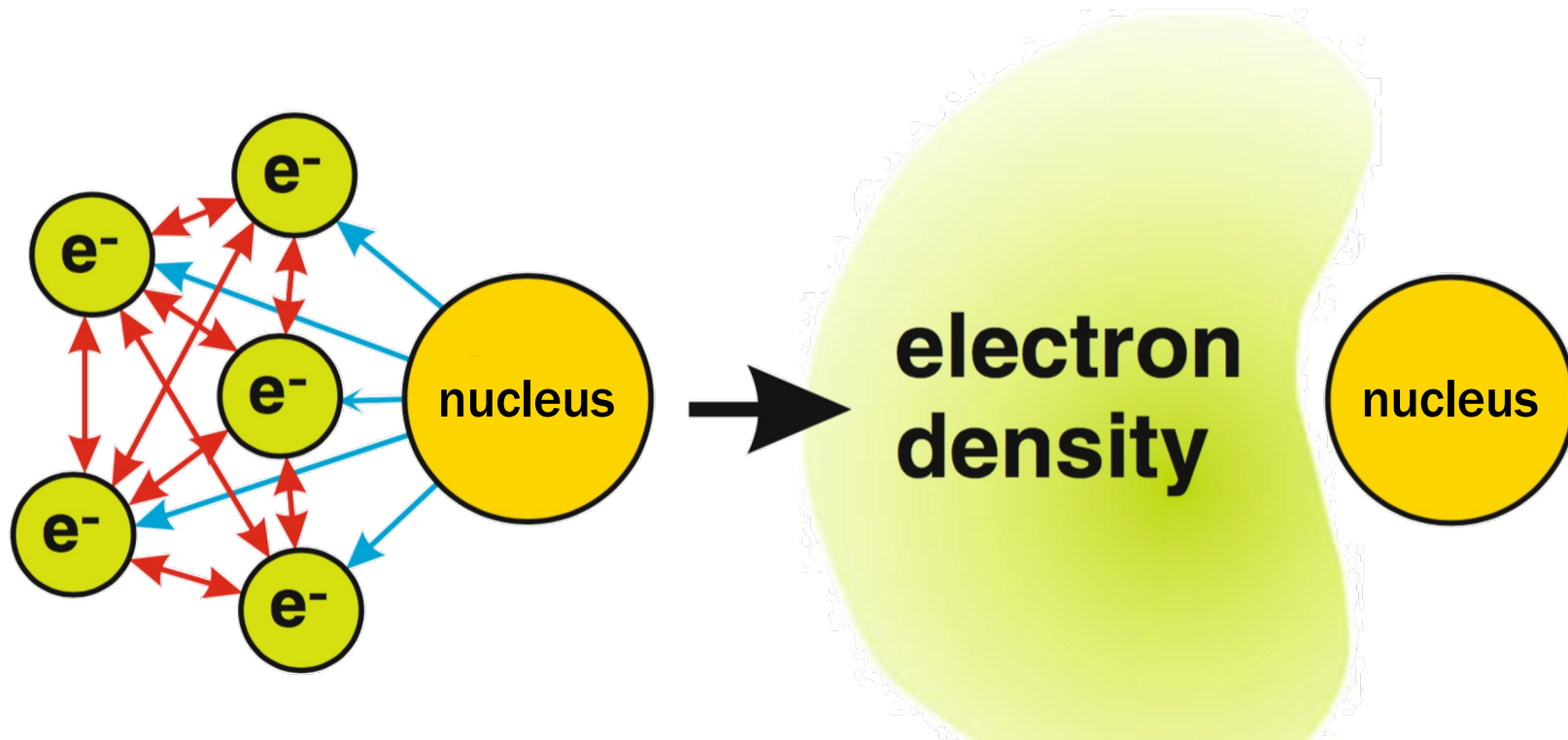


Quantum mechanics of many-electron systems
Paul Dirac, 1929



1950s: Quantum Breakthrough!

Density Functional Theory



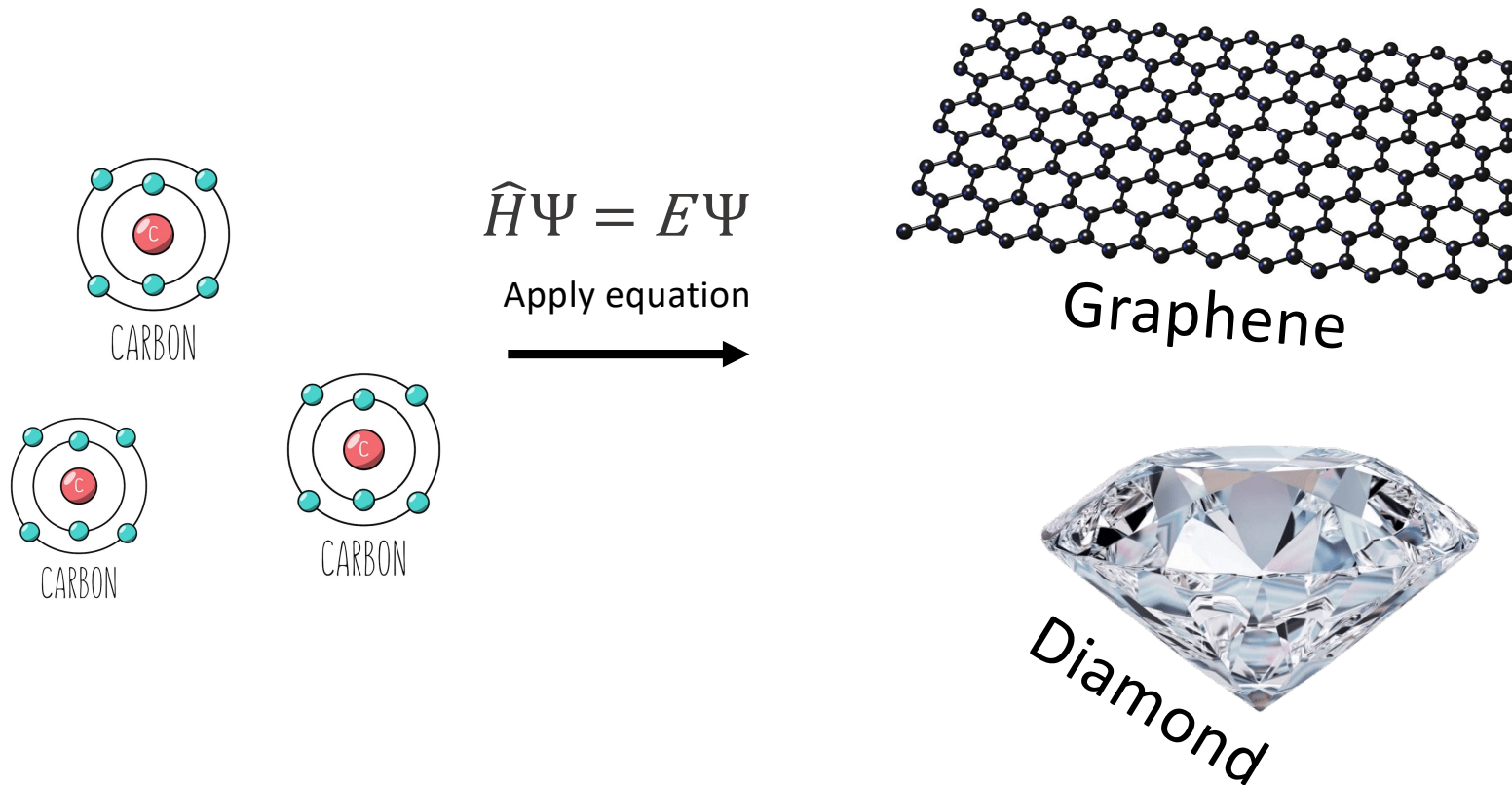
21st Century: Quantum Breakthrough! Supercomputing



Installation of the UK Supercomputer “Archer2”
750,000 compute cores



In Silico materials modelling



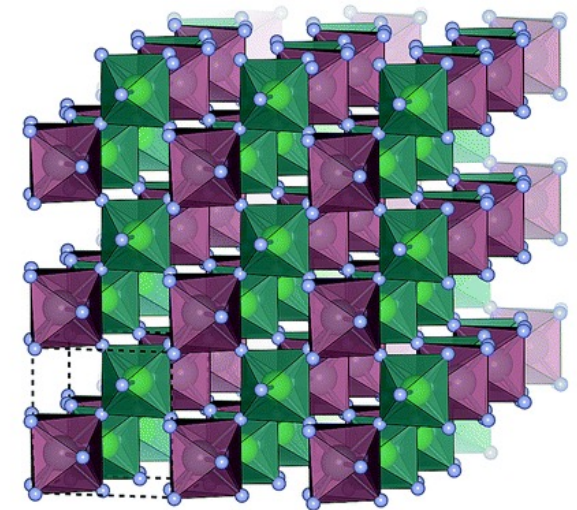
In Silico materials design

1 H																	2 He														
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne														
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar														
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr														
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe														
55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og														

57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No

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

Apply equation



New material!

YZrF7



“The era of global boiling has arrived”

[Antonio Guterres, UN secretary general]

We need new materials for energy conversion and storage



More efficient solar cells



Lighter wind-turbine blades



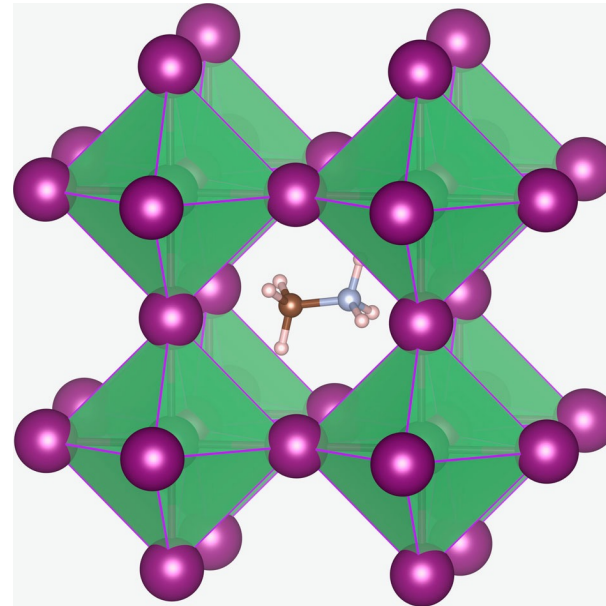
Energy dense batteries



Perovskite: a super-material for solar cells?



inorganic
1839



organic and inorganic
2009



Perovskite: a record-breaking material

Tech

'Miracle material' smashes solar panel efficiency threshold

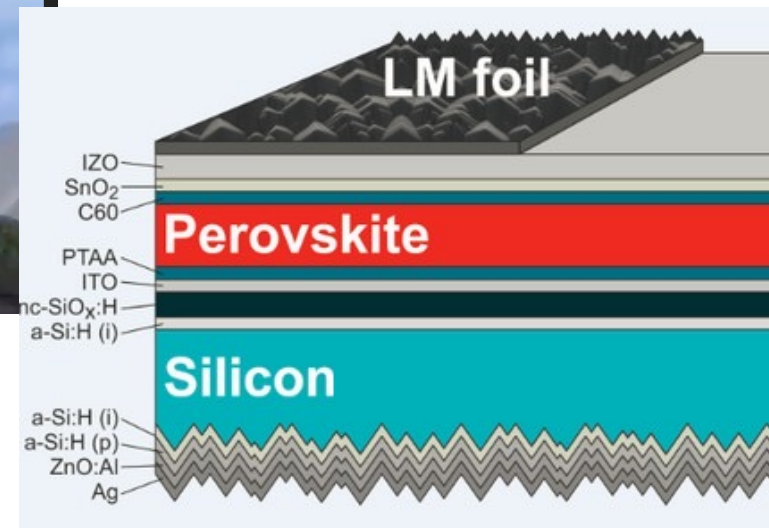
Breakthrough paves way for mass-production of ultra-efficient perovskite solar cells

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

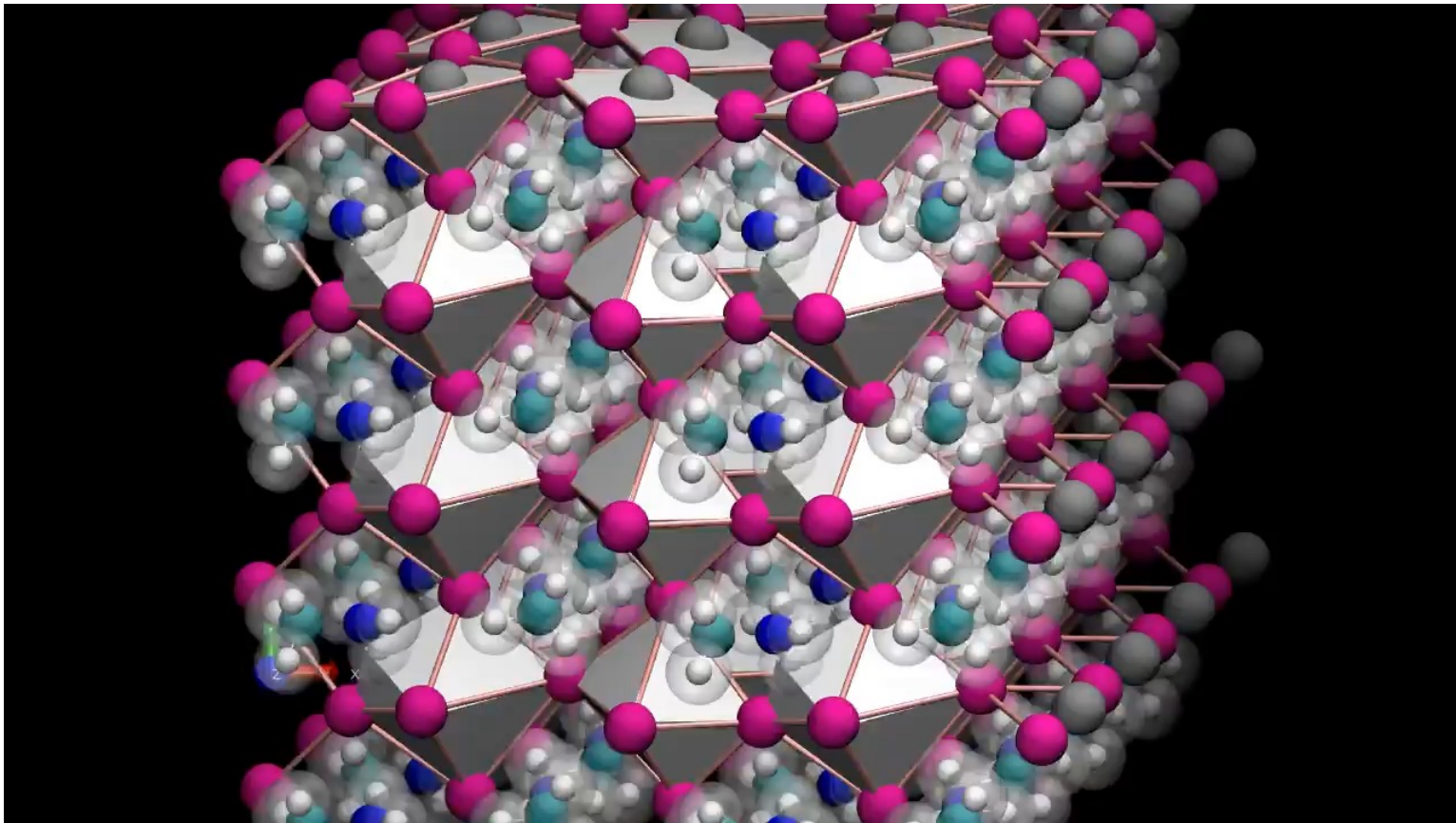


Silicon only → Perovskite on silicon

29% → 33%



Singing Materials



Courtesy Dr Jarvist Frost, Imperial College London



Thanks for listening to me and my materials

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