UNIVERSITY OF CAMBRIDGE

Materials design with artificial intelligence

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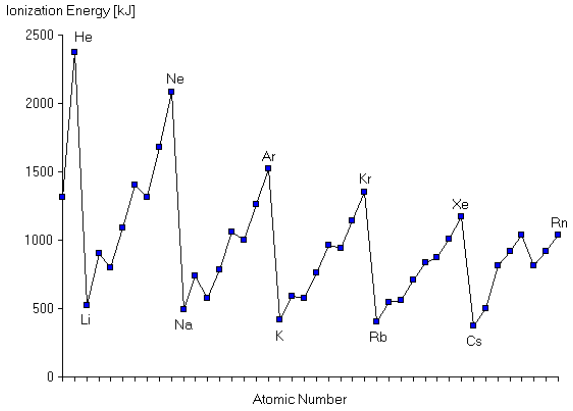
TCM Group, Department of Physics

Approaches to materials design



Experiment

Physical laws

Computer simulation

Materials design

A deep neural network algorithm that

Reduces product development costs

Accelerates product to market

Generic with **proven** applications in materials discovery and drug design

Neural networks: first train

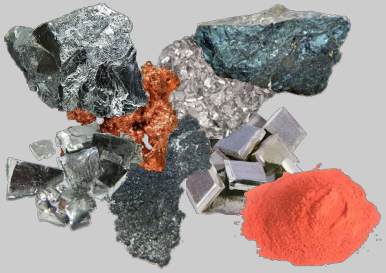
Neural networks: then predict

Unique neural network: train on fragmented data

Unique neural network: predict on fragmented data

Neural networks for materials design

Composition



Artificial intelligence

Properties

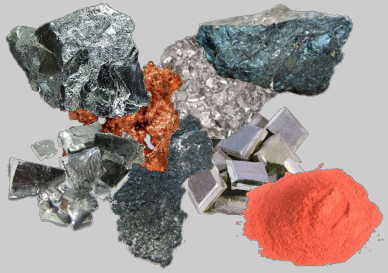
UTS

Hardness

Cost

Neural networks for materials design

Composition



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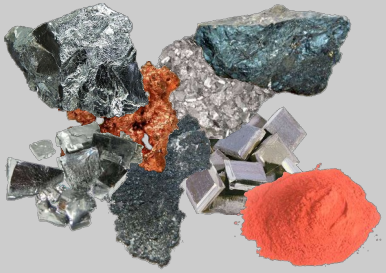

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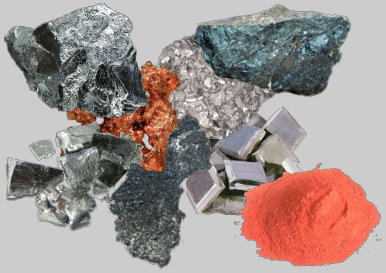


Properties

UTS

Hardness

Cost

Simulations

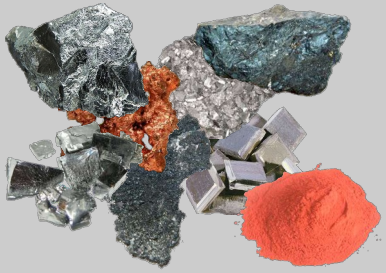
Density Functional

Molecular dynamics

Finite element

Artificial intelligence

Composition



Properties

UTS

Hardness

Cost

Simulations

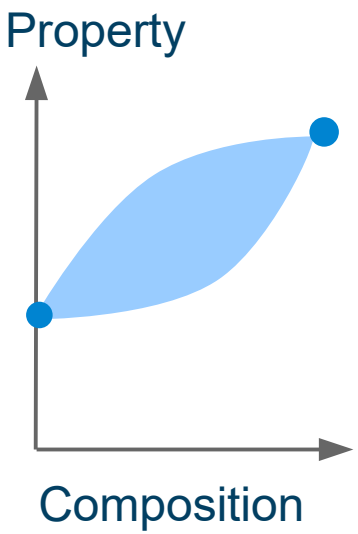
Density Functional

Molecular dynamics

Finite element

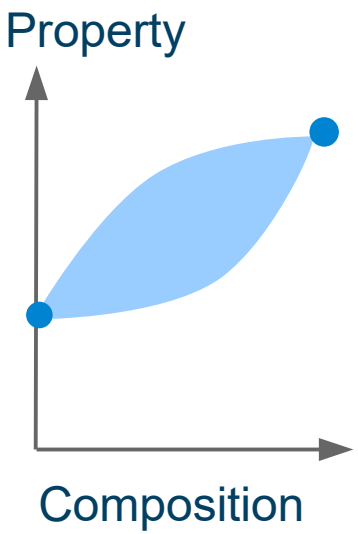
Combine databases with neural networks

Experiment

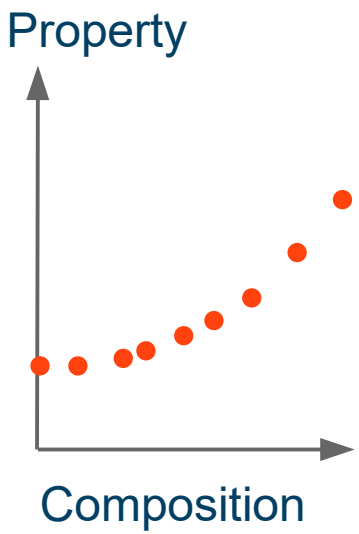


Combine databases with neural networks

Experiment



Simulation

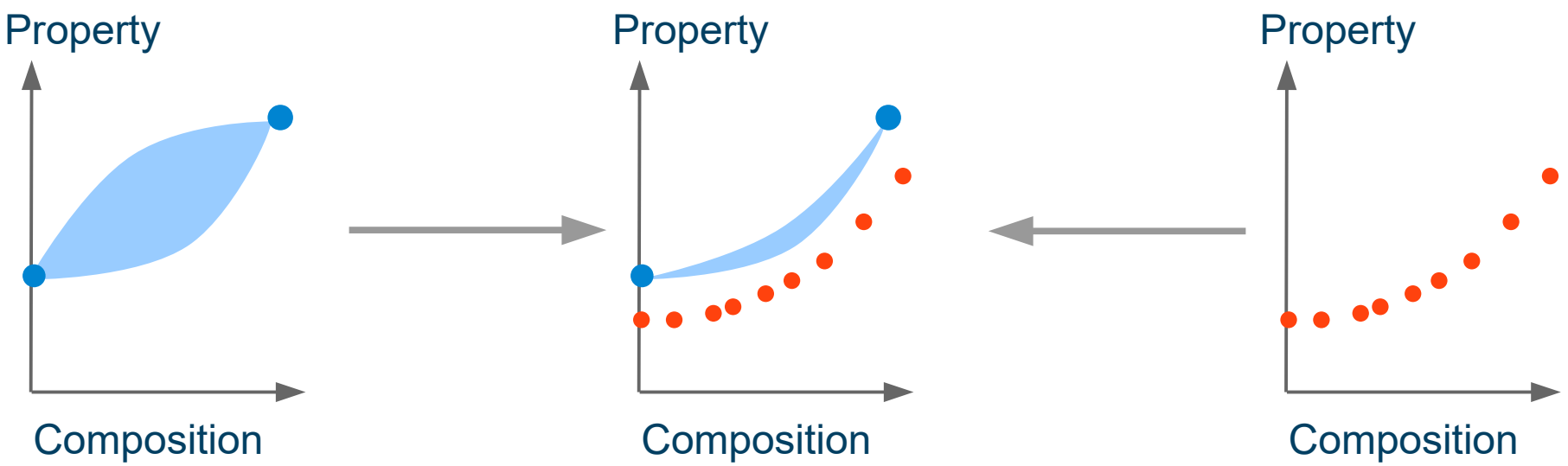


Combine databases with neural networks

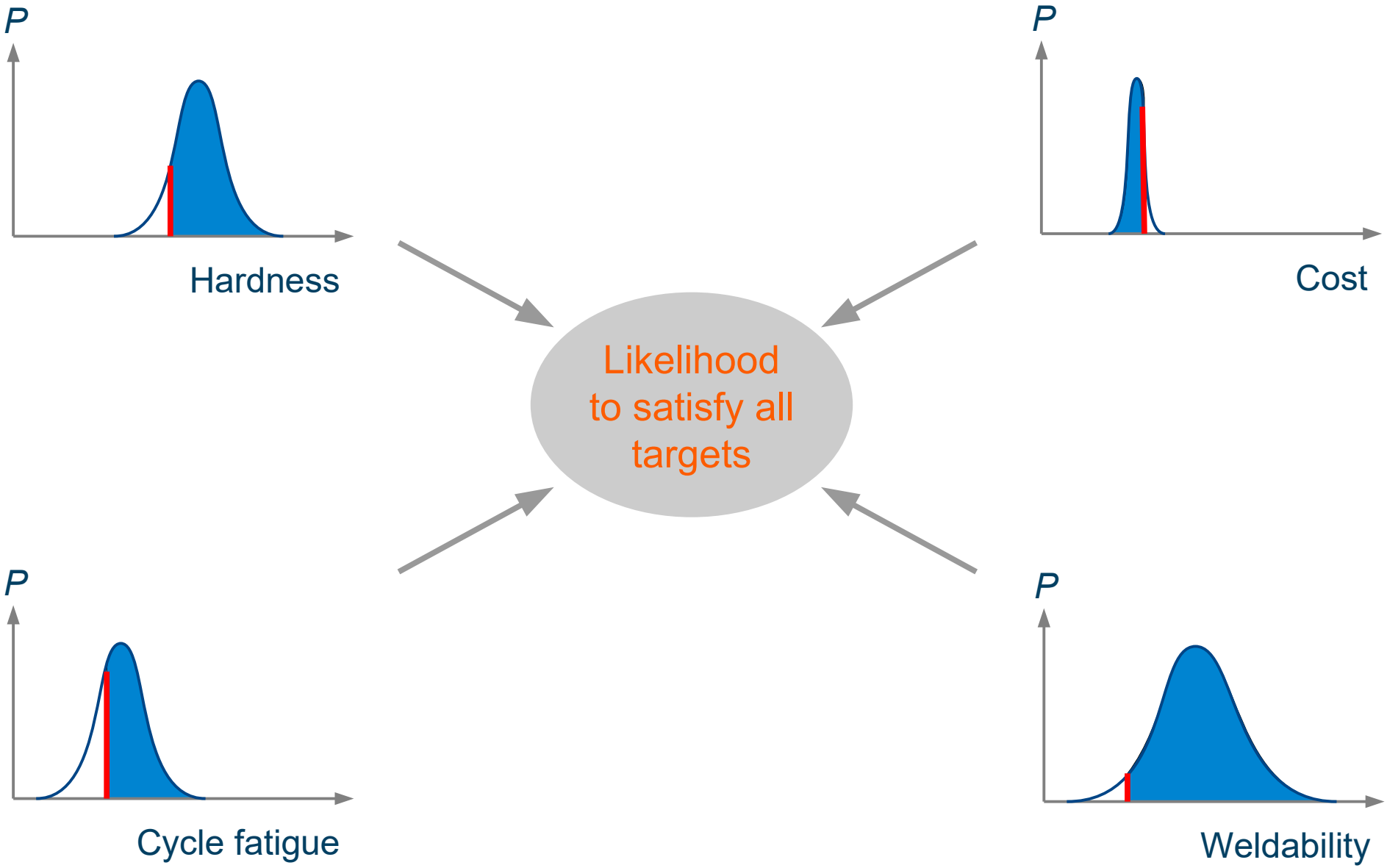
Experiment

Combined

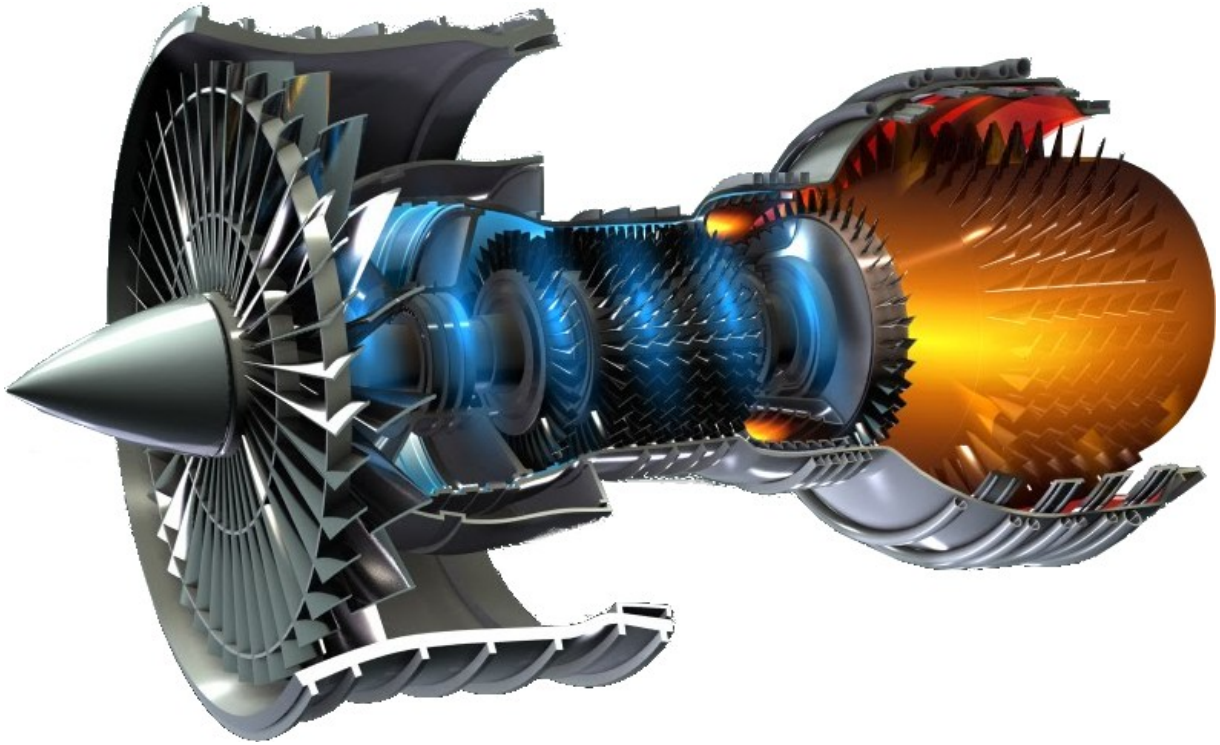
Simulation



Combining likelihood



Schematic of an engine



Target properties

Cost	< 33.7 $\$kg^{-1}$
Density	< 8281 kgm^{-3}
γ’ content	< 50.4 vol%
Phase stability	> 99.0 vol%
Fatigue life	> $10^{3.9}$ cycles
Yield stress	> 752.2 MPa
Ultimate tensile strength	> 960.0 MPa
300hr stress rupture	> 674.5 MPa
Cr activity	> 0.14
γ’ solvus	> 983ºC
Tensile elongation	> 11.6%

Proposed alloy

Cr:15.8

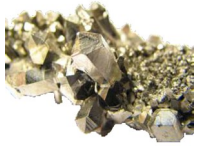
Co: 20.0

Mo: 0.5

W: 0.5

Ta: 4.9

Nb: 1.1



Al: 2.4

Ti: 3.0

Fe: 3.9

Mn: 0.2

Si: 0.2

C: 0.02

B: 0.06

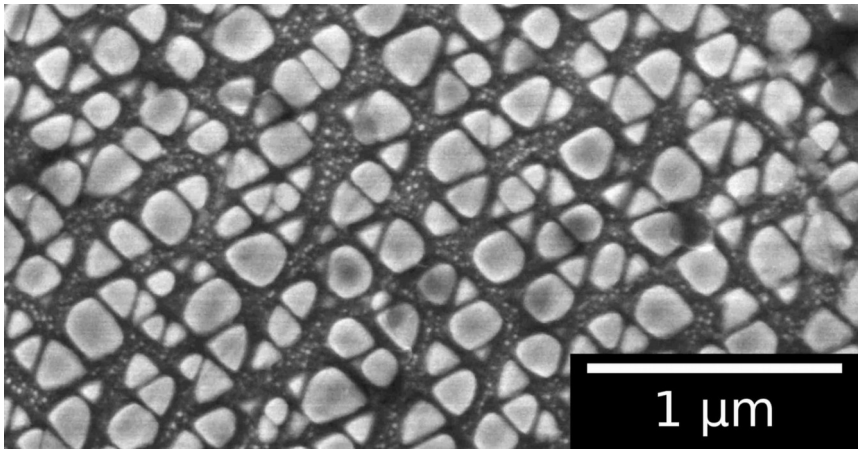
Zr: 0.18

Ni: 47.2

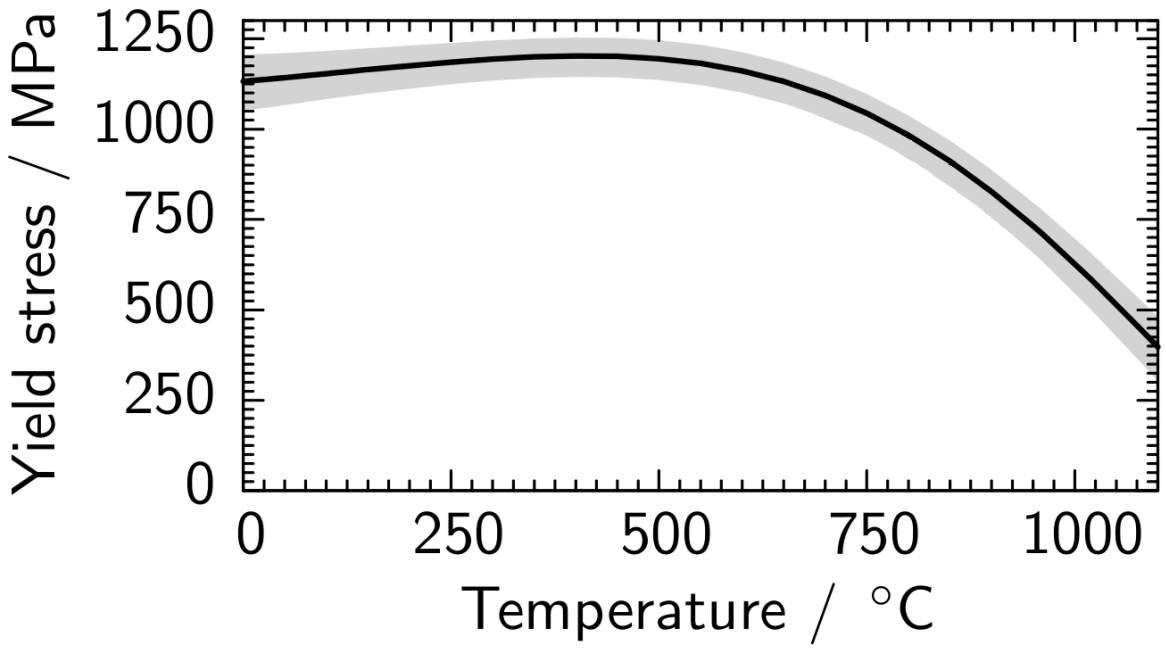
900ºC

30 hours

Microstructure

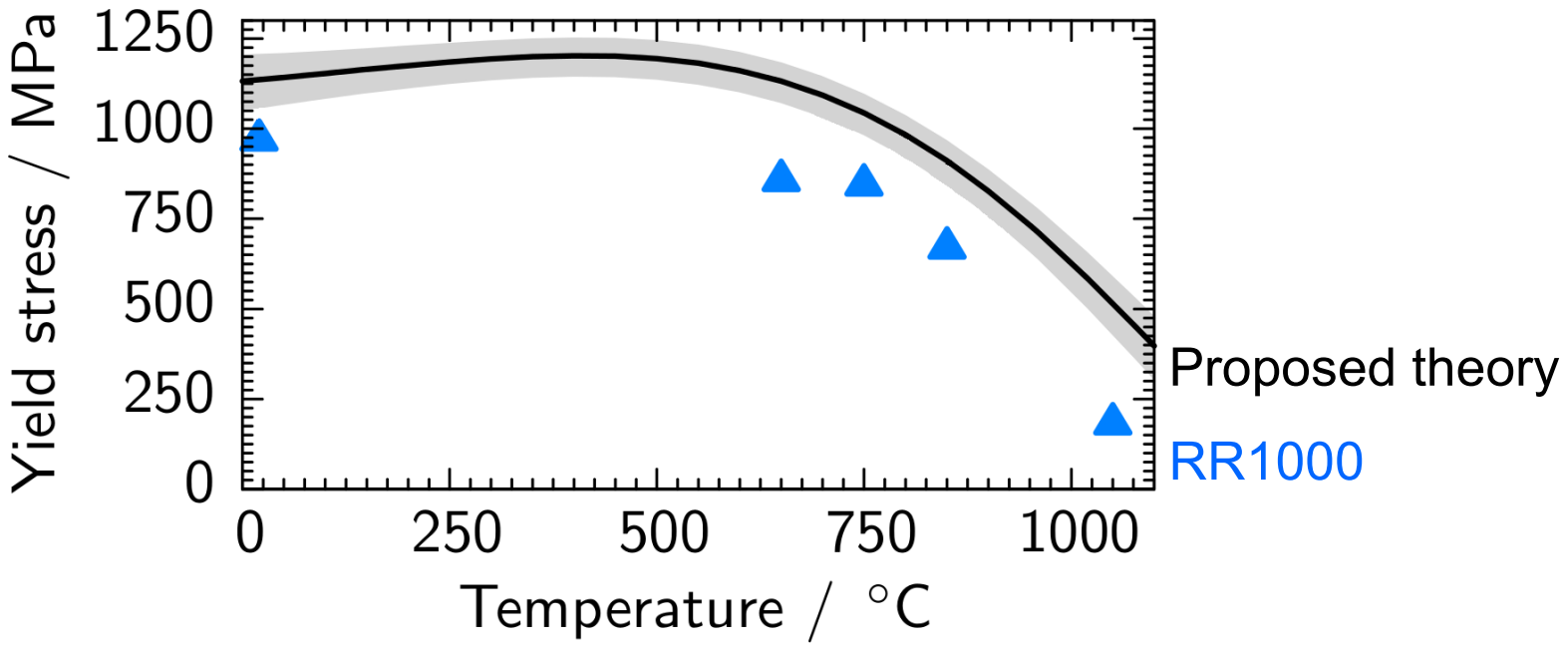


Testing the yield stress

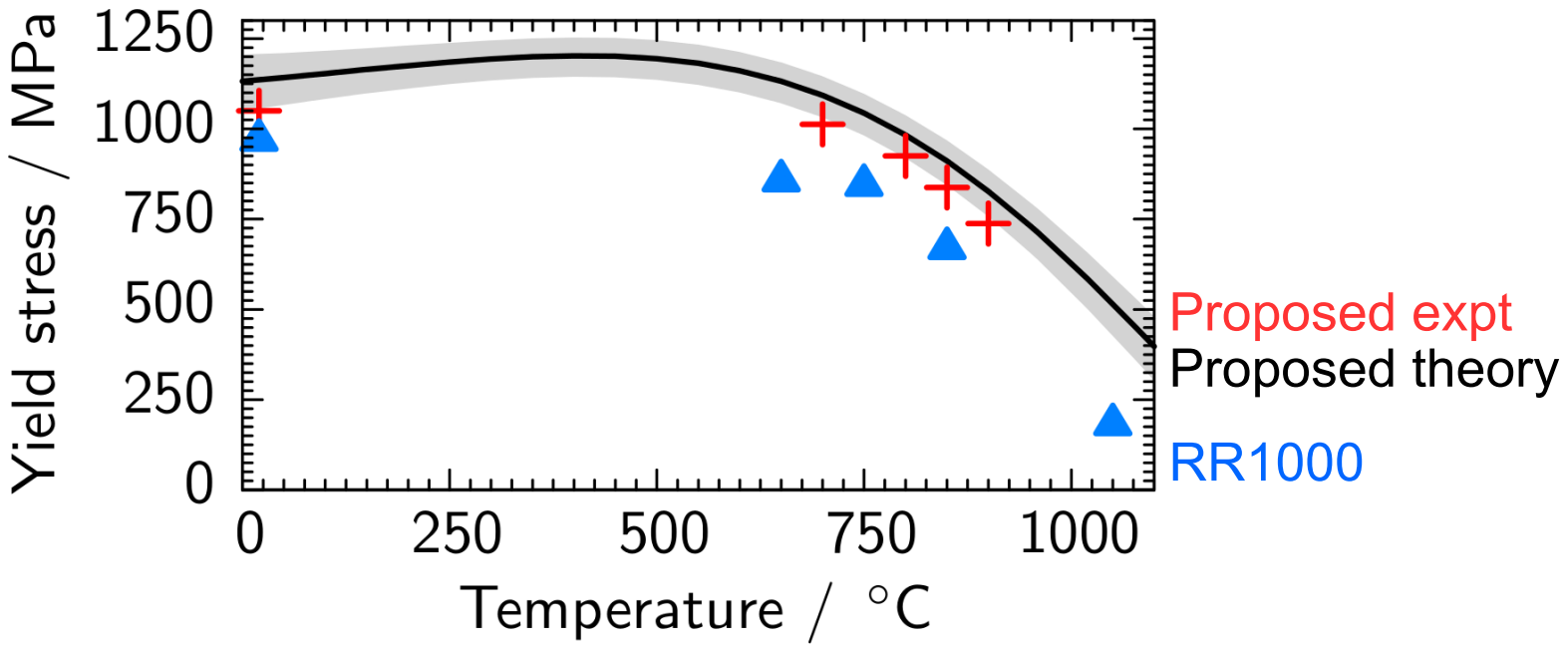


Proposed theory

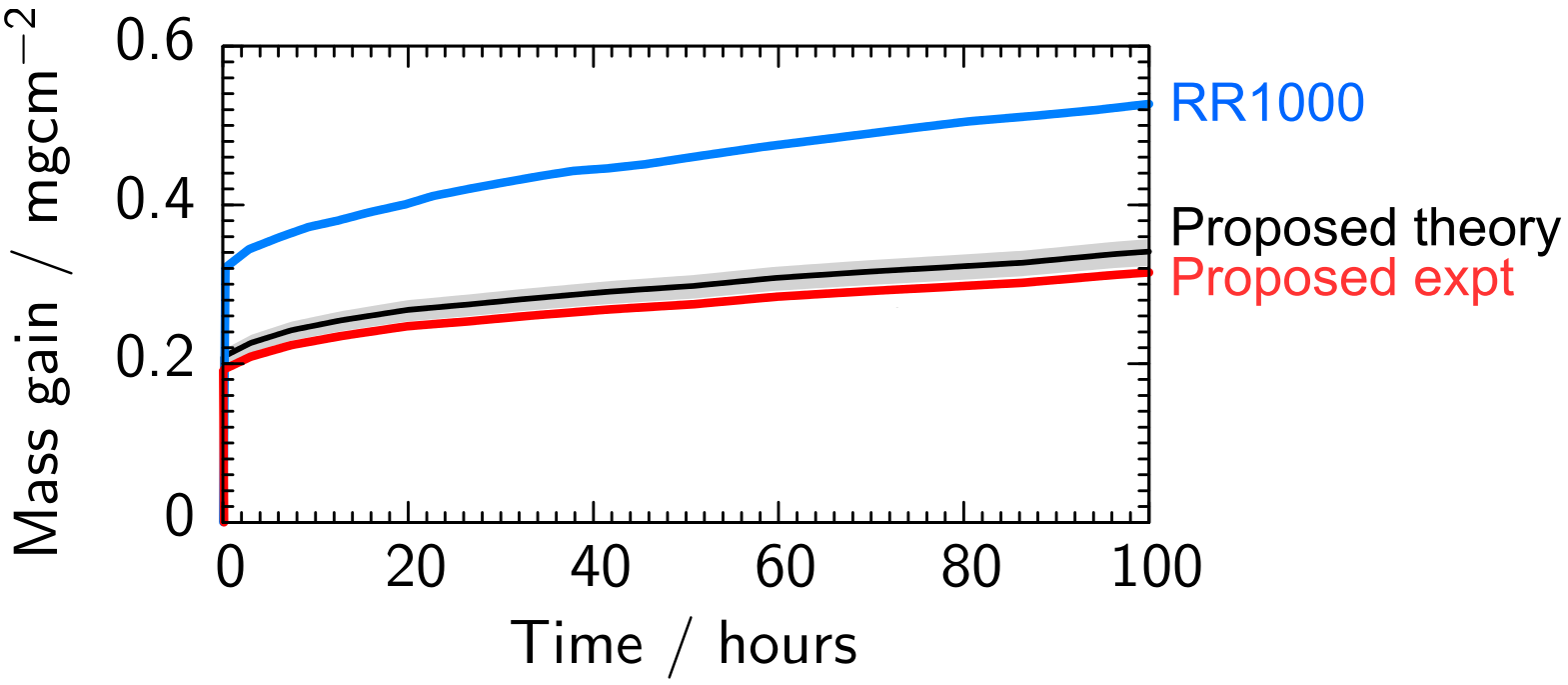
Testing the yield stress



Testing the yield stress

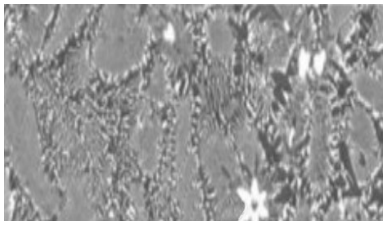


Testing the oxidation resistance

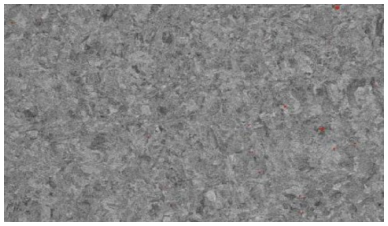


High temperature alloys discovered

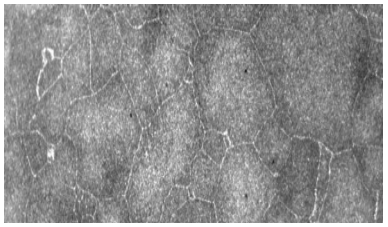
Cr-Cr_2Ta alloys
Intermetallics, 48, 62



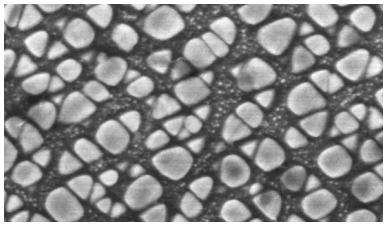
Combustor alloy
GB1408536



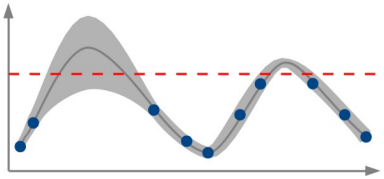
RR1000 grain growth
Acta Materialia, 61, 3378



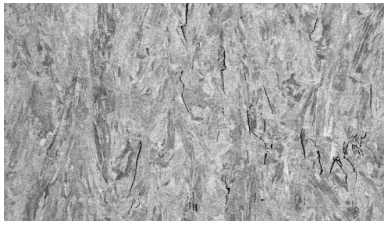
Ni alloy
Materials & Design, 131, 258



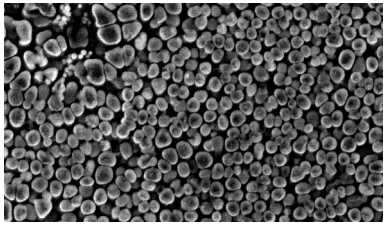
Discovery algorithm
EP14153898
US 2014/177578



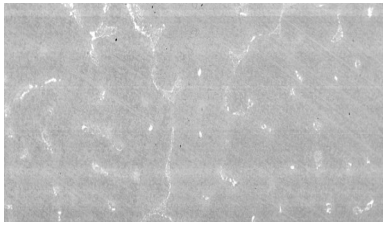
Ni alloy for additive manufacture



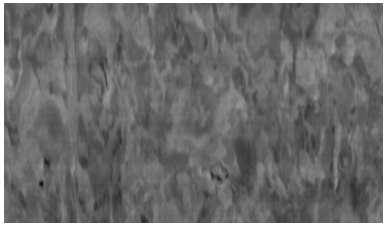
Ni disc alloy
EP14157622
US 2013/0052077 A2



Mo-Hf forging alloy
EP14161255
US 2014/223465

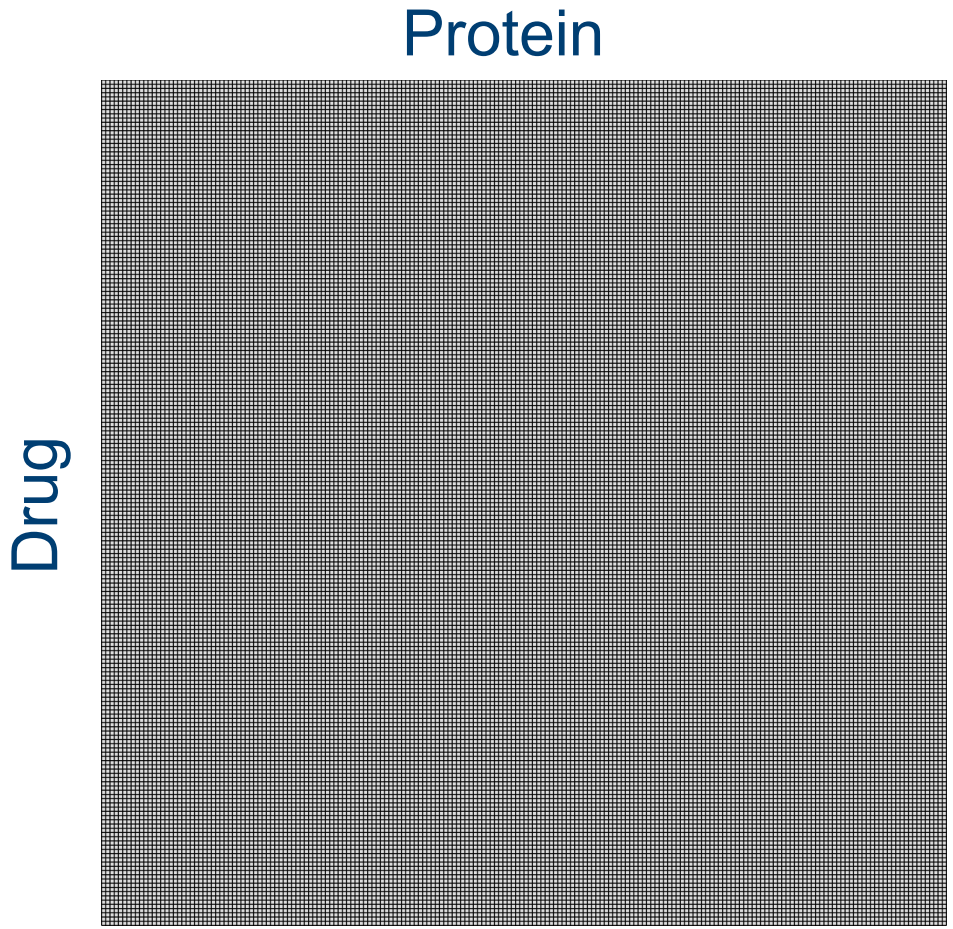


Mo-Nb forging alloy
EP14161529
US 2014/224885



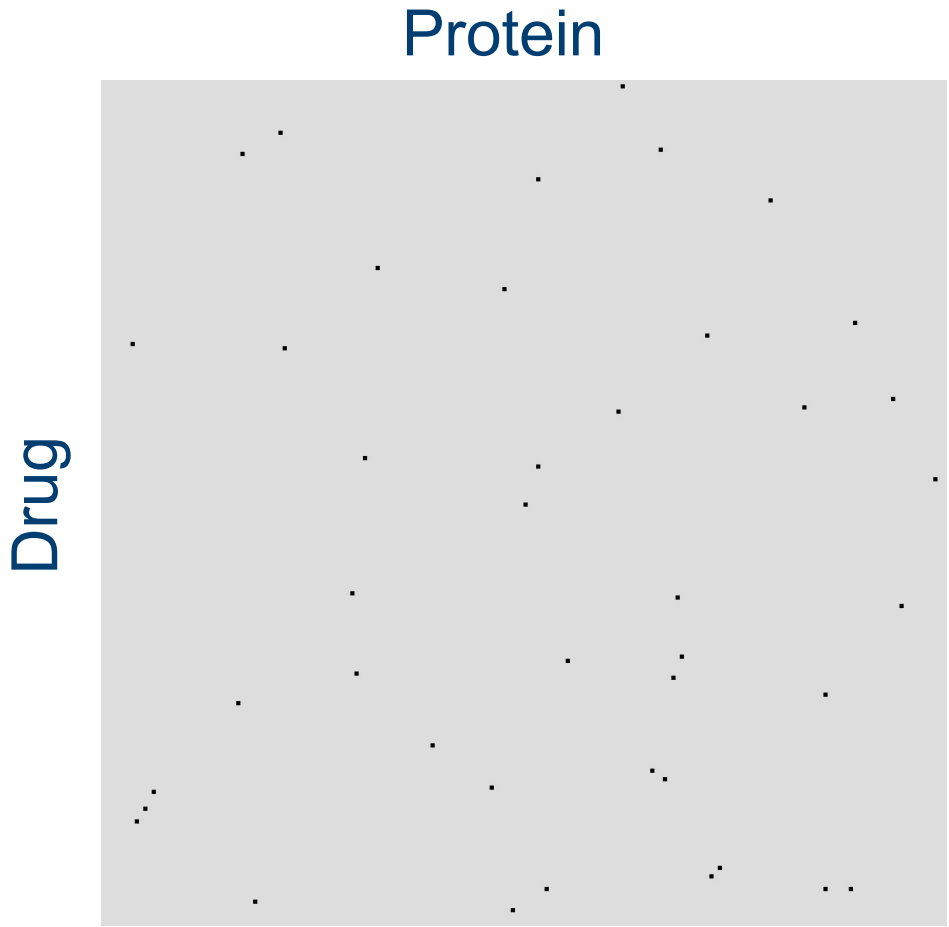
Protein activity database

Database contains 10,000 proteins and 2,000,000 compounds



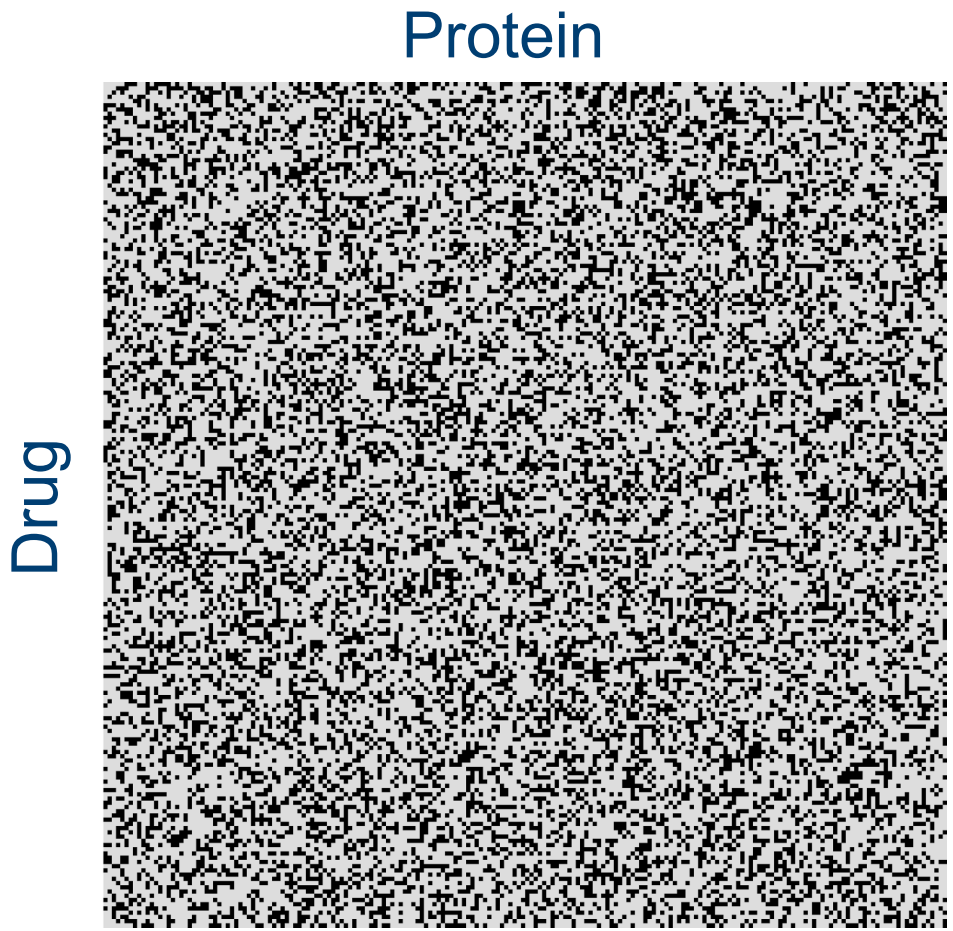
Protein activity data

Database has protein activity for 0.1% of entries



Protein activity data

Filled in 32% of the data points with 75% accuracy



Drug discovery

Data for protein activity with compound

e-therapeutics

Drug discovery

Data for protein activity with compound

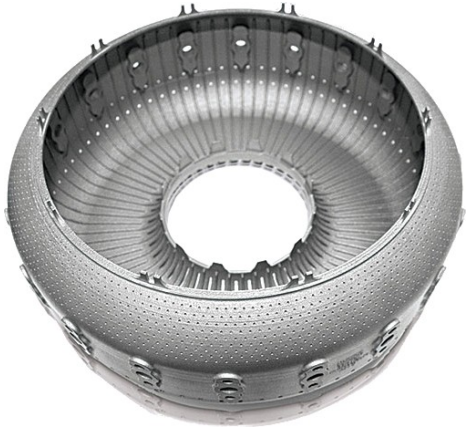
Include additional information about drug structure

Increased drug data available 400-times,
saving $1billion in experimental costs

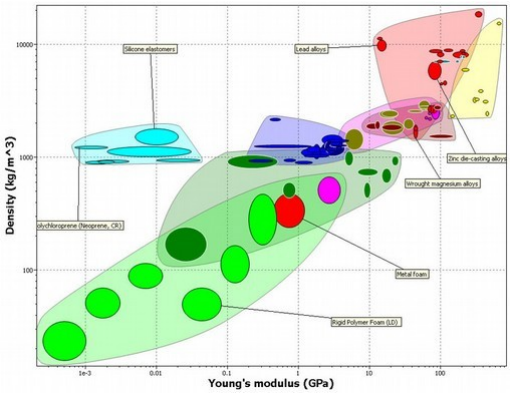
e-therapeutics

Materials design

3D printed alloy
for combustors
Designed from
7 data points



Materials databases
Found 792 errors

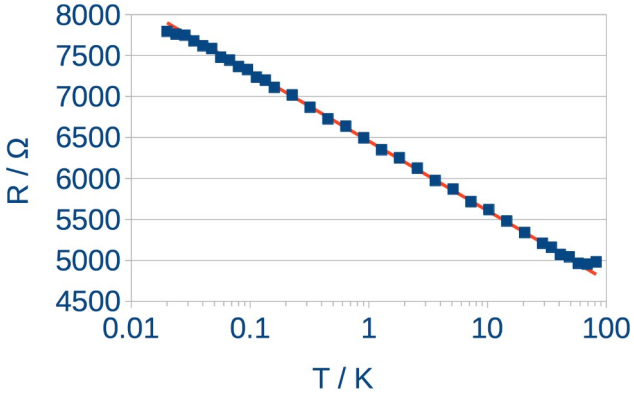


Materials design

Battery design with DFT and experimental data

Designing lubricants with DFT and experimental data

Low temperature thermometer



Yang’s research: motivation

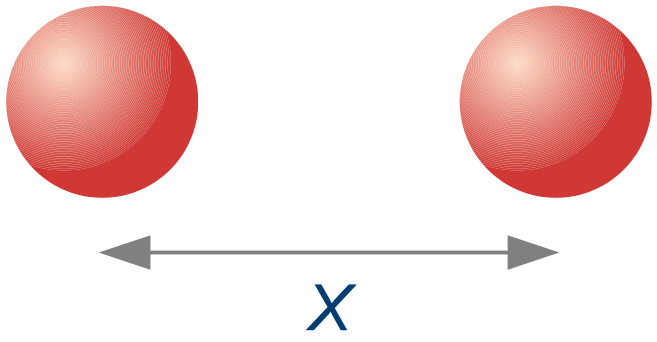
Current first principles computational input to our neural networks is Density Functional Theory

Local density approximation for the energy

Yang's research: the problem

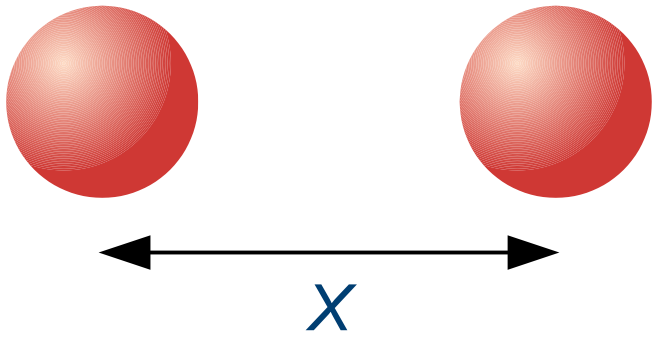
Diffusion Monte Carlo delivers the true ground state electronic wave function, so captures the van der Waals dispersion force

Cannot calculate d^2E/dX^2 so cannot calculate atomic separation and vibrations



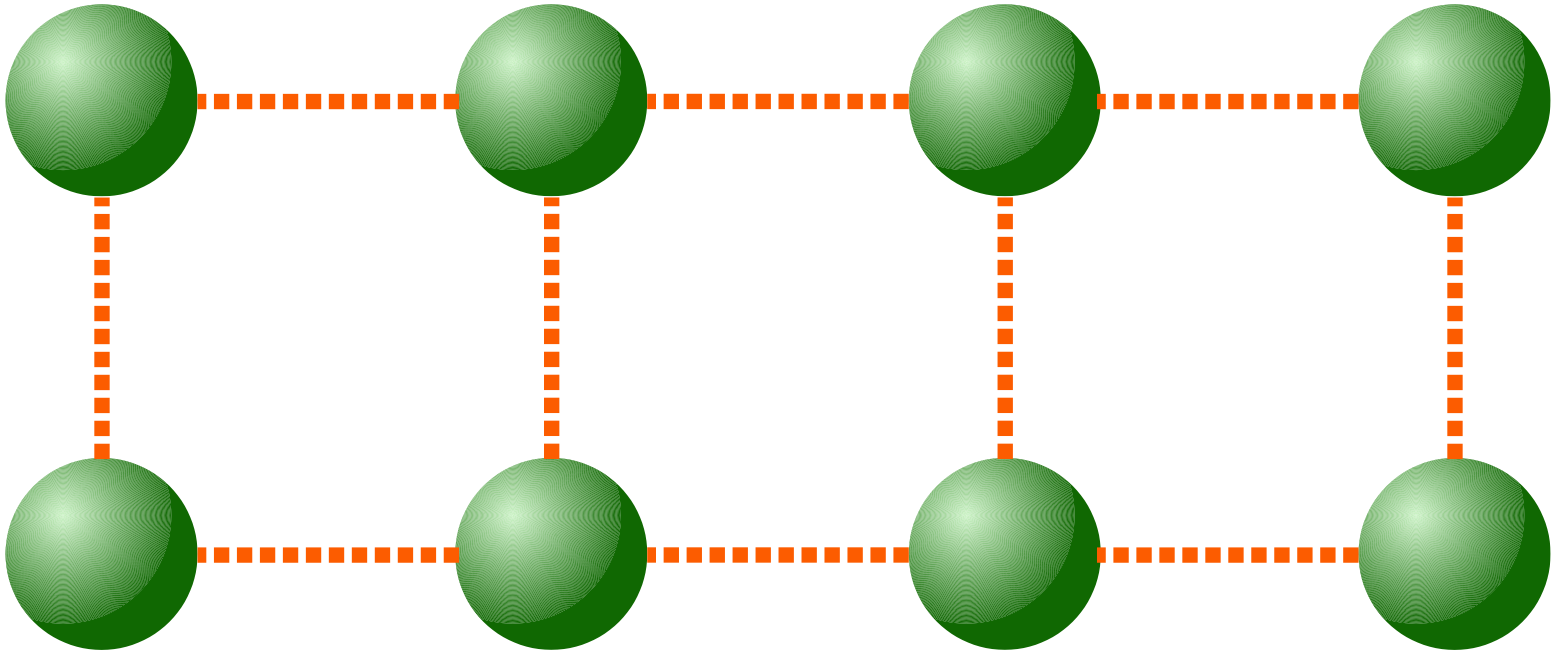
Yang's research: the solution

Implemented the expectation value $\langle d^2H/dX^2 \rangle$. Can calculate atomic separation, vibrational modes, and phonon modes



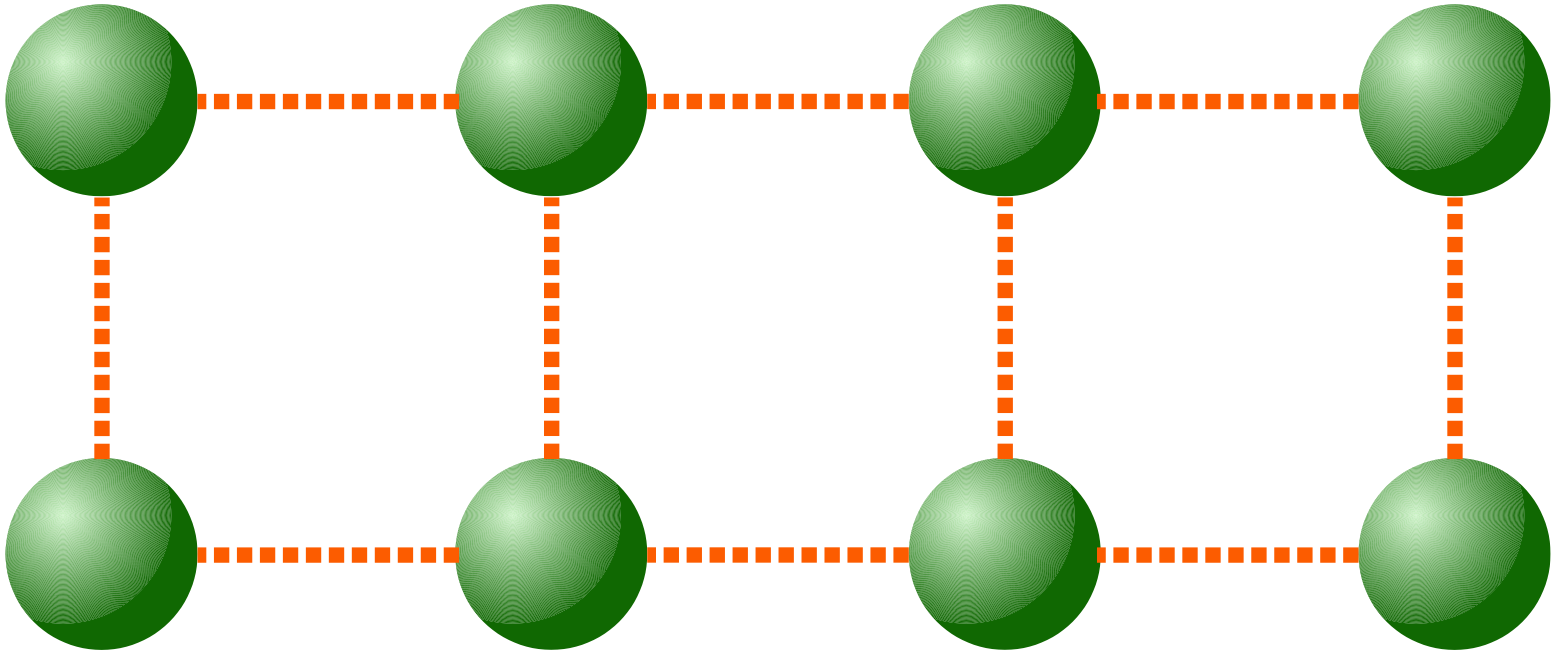
Yang's research: model interatomic bonds as springs

Ions repel like springs to give harmonic vibrations



Yang's research: contributions to interatomic bonds

$$\langle\, d^2H/dX^2 \,\rangle \;=\; \langle\, d^2V_{\text{ion-ion}}/dX^2 + d^2V_{\text{elec-ion}}/dX^2 + 2dV_{\text{elec-ion}}/dX\,d\psi/dX \,\rangle$$



Yang's research: surprising insight about phonons

$d^2V_{ion\text{-}ion}/dX^2=0$ in simple cubic, FCC, BCC, wurtzite, diamond structures

Yang's research: stability of crystals

$d^2V_{ion\text{-}ion}/dX^2=0$ in simple cubic, FCC, BCC, wurtzite, diamond structures

In tight binding systems $\langle dV_{elec\text{-}ion}/dX d\psi/dX \rangle$ is small and $\langle d^2V_{elec\text{-}ion}/dX^2=-Ar^2 \rangle$, an instability

Yang's research: stability of crystals

$d^2E/dX^2<0$ in tight binding simple cubic, FCC, BCC, wurtzite, diamond structures

	1 H HEX																2 He HCP
	3 Li BCC	4 Be HCP											5 B RHO	6 C HEX	7 N HEX	8 O SC	9 F SC	10 Ne FCC
	11 Na BCC	12 Mg HCP											13 Al FCC	14 Si DC	15 P ORTH	16 S ORTH	17 Cl ORTH	18 Ar FCC
	19 K BCC	20 Ca FCC	21 Sc HCP	22 Ti HCP	23 V BCC	24 Cr BCC	25 Mn BCC	26 Fe BCC	27 Co HCP	28 Ni FCC	29 Cu FCC	30 Zn HCP	31 Ga ORTH	32 Ge DC	33 As RHO	34 Se HEX	35 Br ORTH	36 Kr FCC
	37 Rb BCC	38 Sr FCC	39 Y HCP	40 Zr HCP	41 Nb BCC	42 Mo BCC	43 Tc HCP	44 Ru HCP	45 Rh FCC	46 Pd FCC	47 Ag FCC	48 Cd HCP	49 In TETR	50 Sn TETR	51 Sb RHO	52 Te HEX	53 I ORTH	54 Xe FCC
	55 Cs BCC	56 Ba BCC	57* La DHCP	72 Hf HCP	73 Ta BCC/TETR	74 W BCC	75 Re HCP	76 Os HCP	77 Ir FCC	78 Pt FCC	79 Au FCC	80 Hg RHO	81 Tl HCP	82 Pb FCC	83 Bi RHO	84 Po SC/RHO	85 At [FCC]	86 Rn FCC
	87 Fr [BCC]	88 Ra BCC	89** Ac FCC	104 Rf [HCP]	105 Db [BCC]	106 Sg [BCC]	107 Bh [HCP]	108 Hs [HCP]	109 Mt [FCC]	110 Ds [BCC]	111 Rg [BCC]	112 Cn [HCP]	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og [FCC]
*			58 Ce DHCP/FCC	59 Pr DHCP	60 Nd DHCP	61 Pm DHCP	62 Sm RHO	63 Eu BCC	64 Gd HCP	65 Tb HCP	66 Dy HCP	67 Ho HCP	68 Er HCP	69 Tm HCP	70 Yb FCC	71 Lu HCP		
**			90 Th FCC	91 Pa TETR	92 U ORTH	93 Np ORTH	94 Pu MON	95 Am DHCP	96 Cm DHCP	97 Bk DHCP	98 Cf DHCP	99 Es FCC	100 Fm [FCC]	101 Md [FCC]	102 No [FCC]	103 Lr [HCP]		

Summary

Apply deep learning to high-value fragmented data

Cut costs by reducing need for expensive experiments

Discovery and verification in materials and drug discovery

Merge experiments and simulations into holistic design tool

Worked with 7 companies, founded startup intellegens