intellegens

Quantum leap for machine learning

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Materials and pharmaceuticals market

Materials enabler for new technology, advanced materials market estimates at $1.5 trillion per year

Pharmaceuticals at heart of human health, worth $1 trillion per year

Improvements to materials or pharmaceuticals offer significant impact

Ripe for disruption – new formulations found after ~20 years of experimental driven trial and improvement

Challenge of machine learning in experimental sciences

Train from sparse datasets, typically found in experimental sciences

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Steel 1	99.1	0.27	0.6	842	76		149
Steel 2	98.6		0.9			80	170
Steel 3		0.42		1100			179
Steel 4	98.4	0.55	0.8		118	70	

Challenge of machine learning in materials

Train from sparse datasets, typically found in experimental sciences

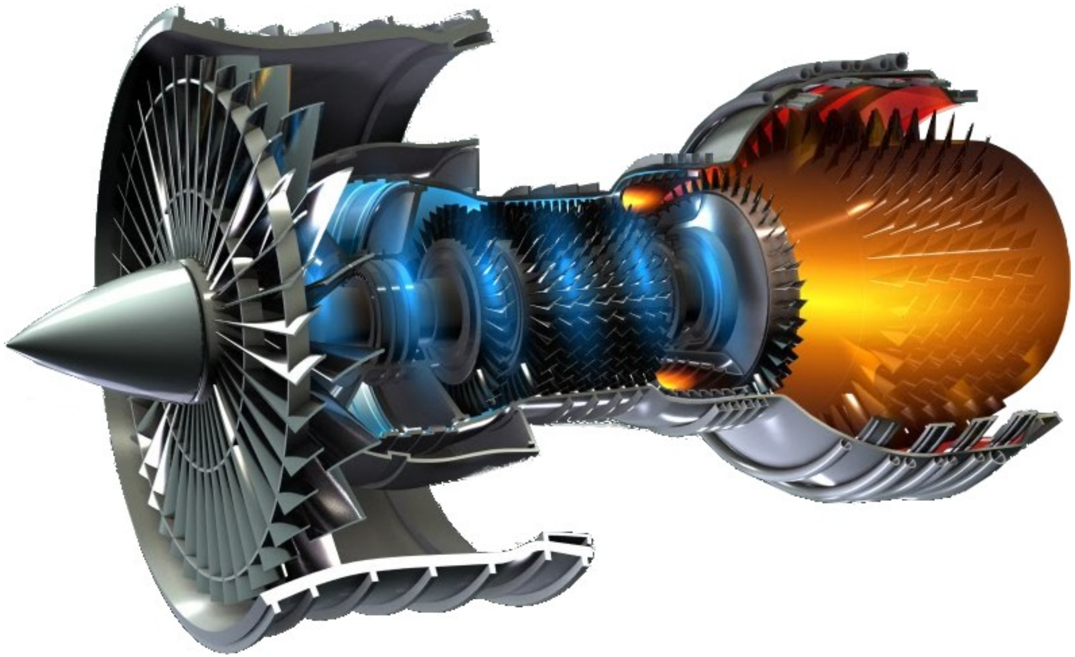
Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

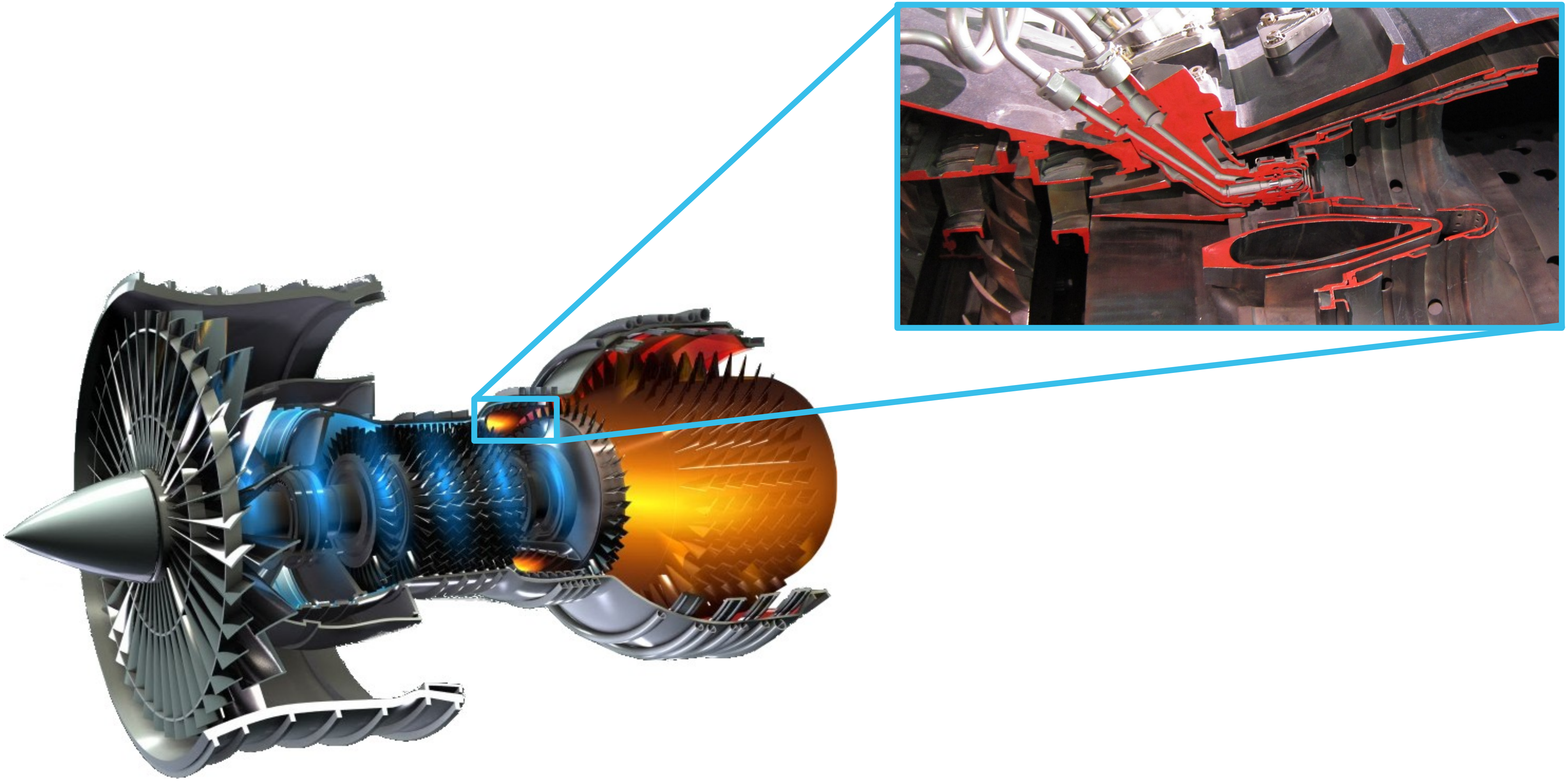
Accelerate discovery of new formulations

Generic with applications in materials and pharmaceuticals

Jet engine



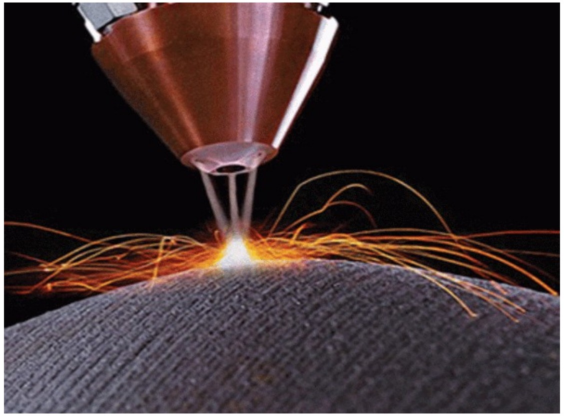
Jet engine combustor



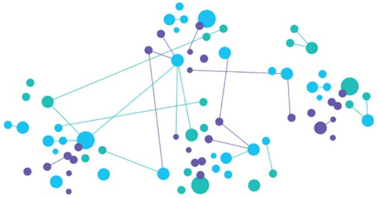
Target properties

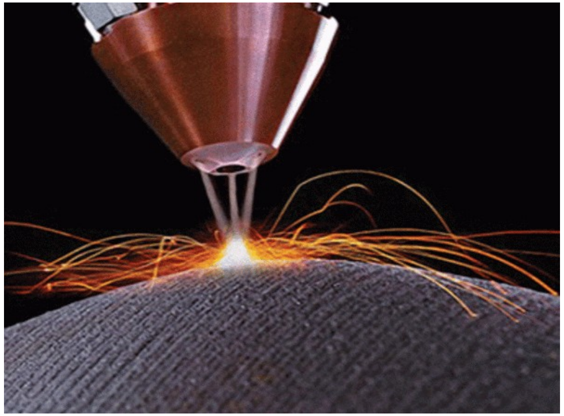
Elemental cost	$< 25\ \$kg^{-1}$
Density	$< 8500\ kgm^{-3}$
γ’ content	< 25 wt%
Oxidation resistance	$< 0.3\ mgcm^{-2}$
Processability	< 0.15% defects
Phase stability	> 99.0 wt%
γ’ solvus	> 1000˚C
Thermal resistance	$> 0.04\ K\Omega^{-1}m^{-3}$
Yield stress at 900˚C	> 200 MPa
Tensile strength at 900˚C	> 300 MPa
Tensile elongation at 700˚C	> 8%
1000hr stress rupture at 800˚C	> 100 MPa
Fatigue life at 500 MPa, 700˚C	$> 10^5$ cycles

Direct laser deposition

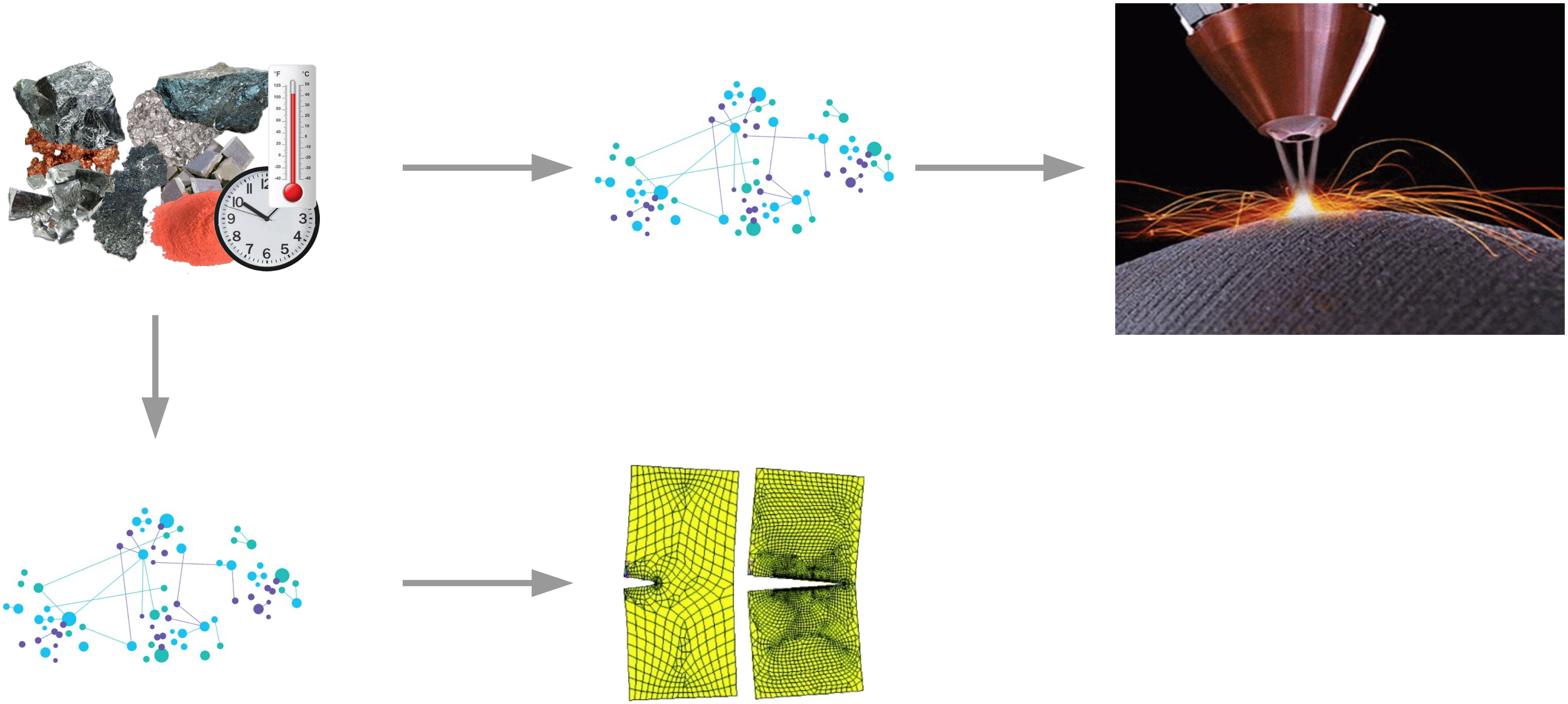


Machine learning prediction of direct laser deposition

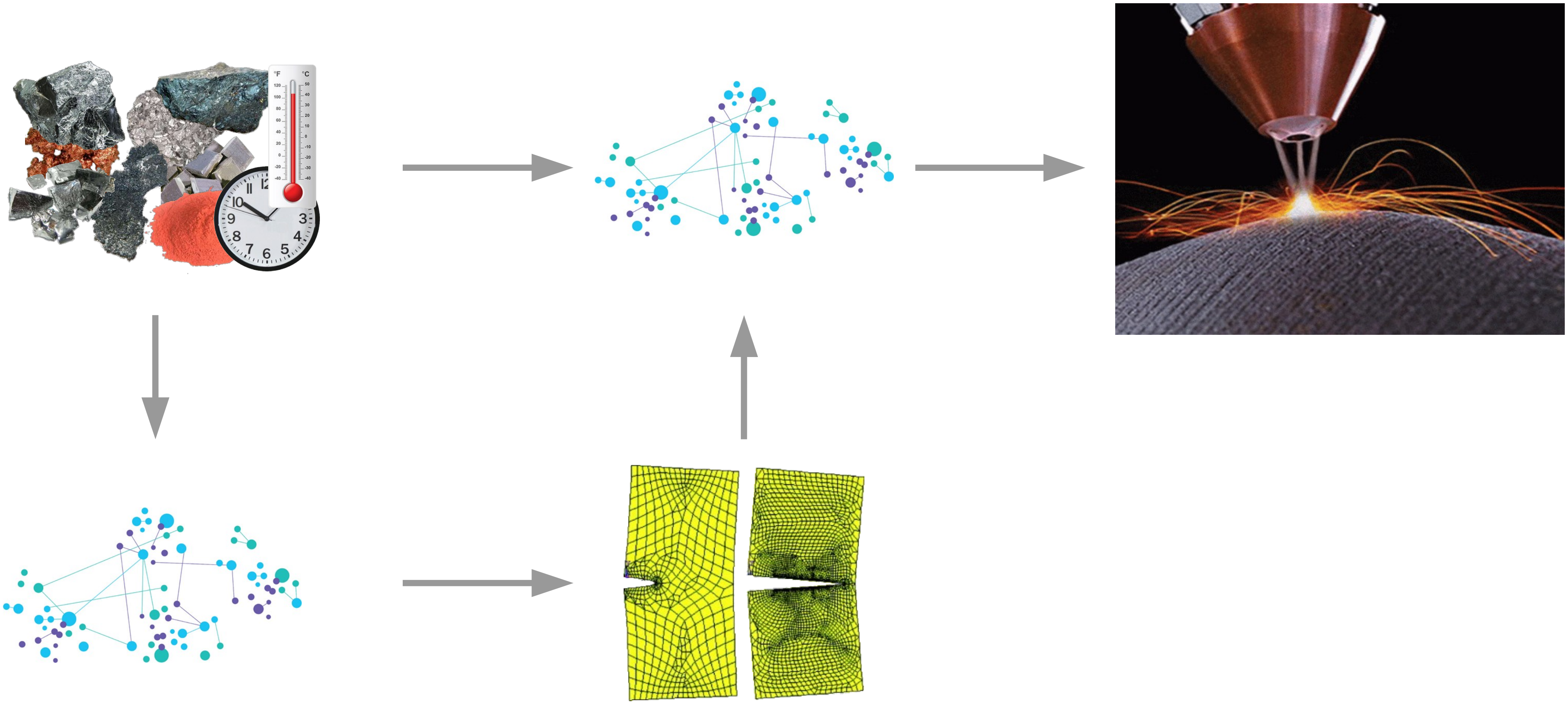




Machine learning prediction of crack formation



Predict direct laser deposition from crack formation



Composition designed

Cr: 19%

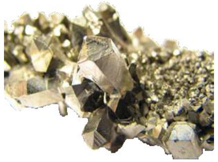
Co: 4%

Mo: 4.9%

W: 1.2%

Zr: 0.05%

Nb: 3%



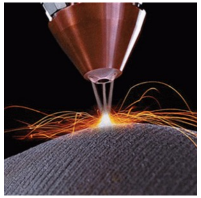
Al: 2.9%

C: 0.04%

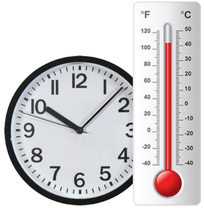
B: 0.01%

Ni

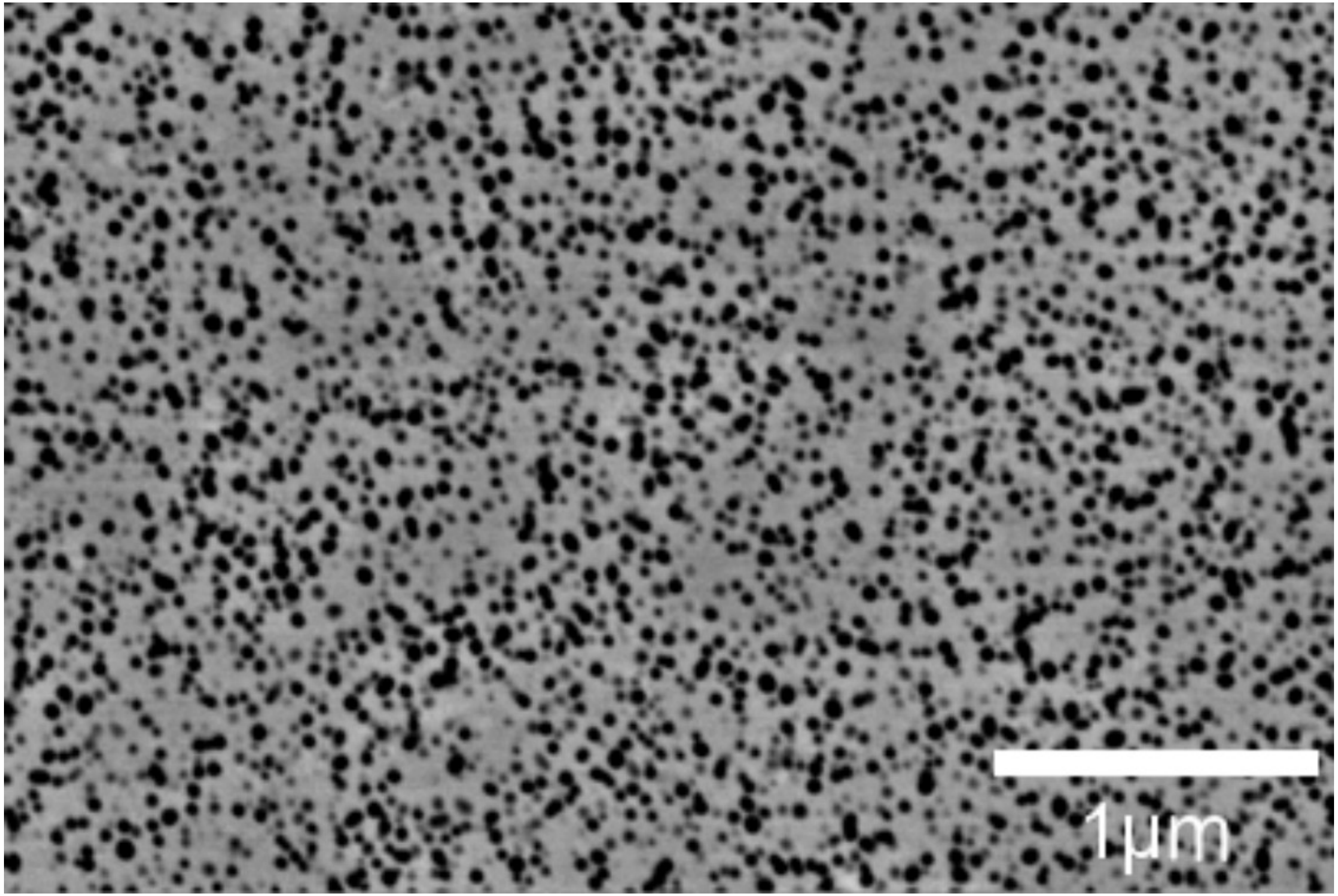
Expose 0.8



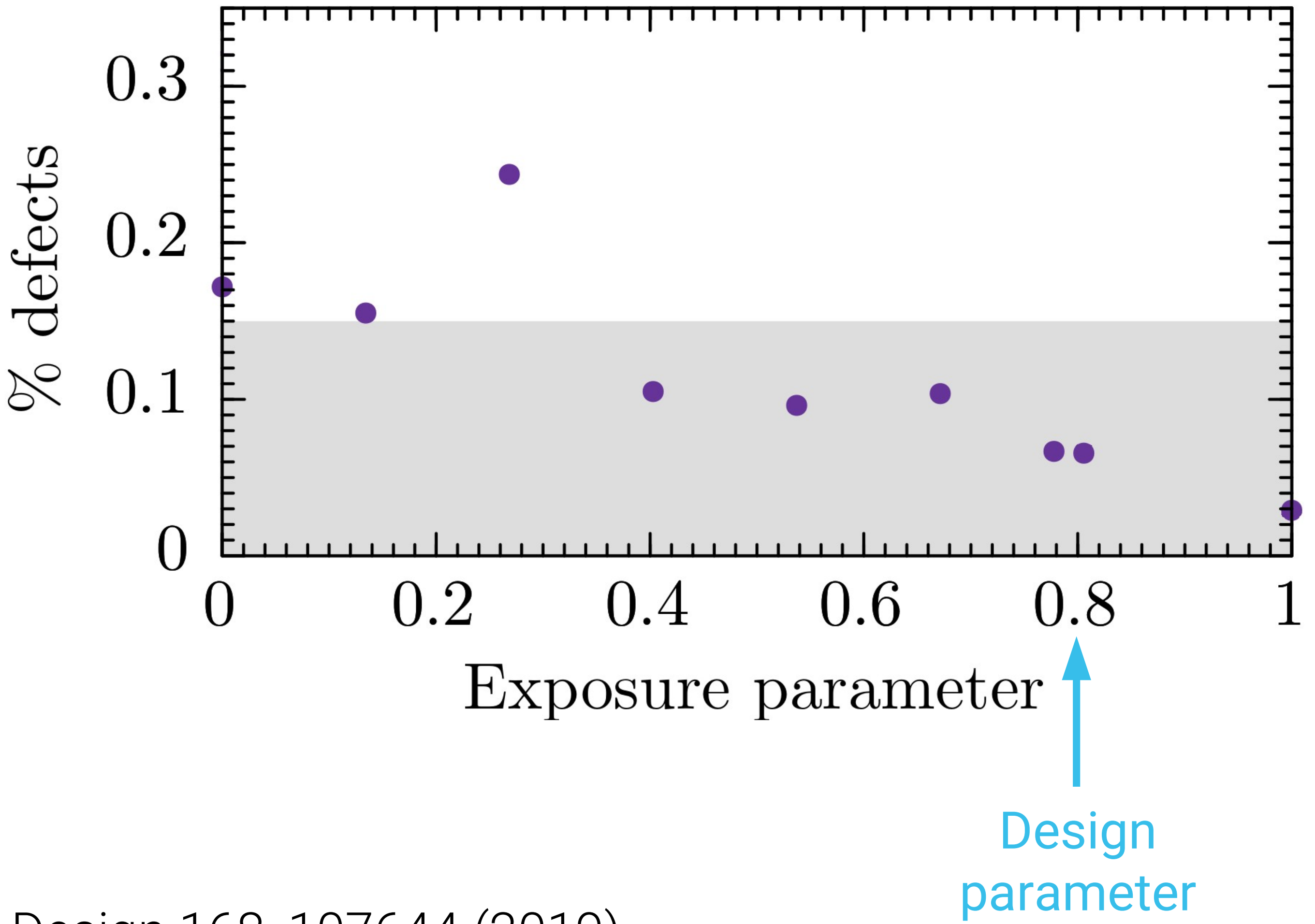
T_{HT} 1300°C



Microstructure



Measuring the defect density



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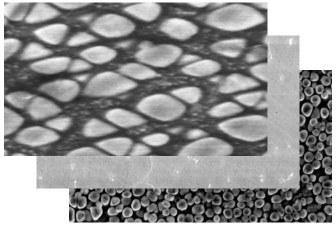
Other materials designed

Nickel and
molybdenum



Steel for welding

Experiment and
DFT for batteries

Other materials designed

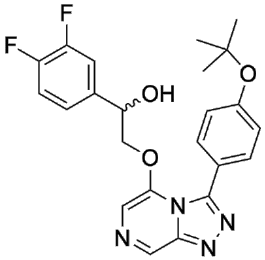
Lubricants with molecular dynamics and experiments

bp

Drug design

e-therapeutics
optibrium
AstraZeneca
Celgene
Takeda
Constellation PHARMACEUTICALS

Open Source Malaria competition



OPEN SOURCE MALARIA
Looking for New Medicines

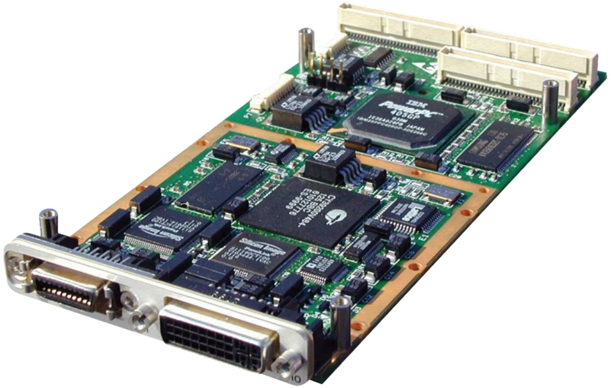
Applications of quantum computing to machine learning

Accelerated implementation of standard algorithms in machine learning

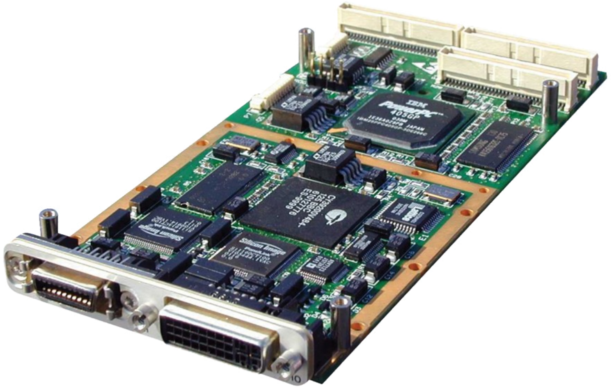
Development of new machine learning methods, quicker and better at handling missing data

Enhance underlying first principles predictions

Specific standard algorithm library improvements



Specific standard algorithm library improvements



Neural network requires matrix multiplication

Random forest requires sorting

Ambitious improvements in machine learning

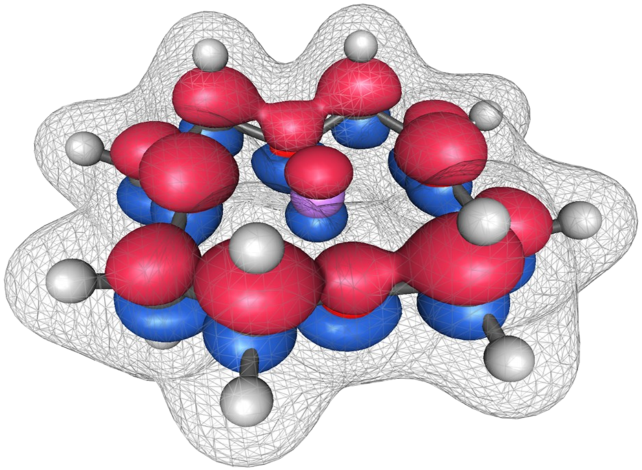
Handling unknown values through superposition of quantum states

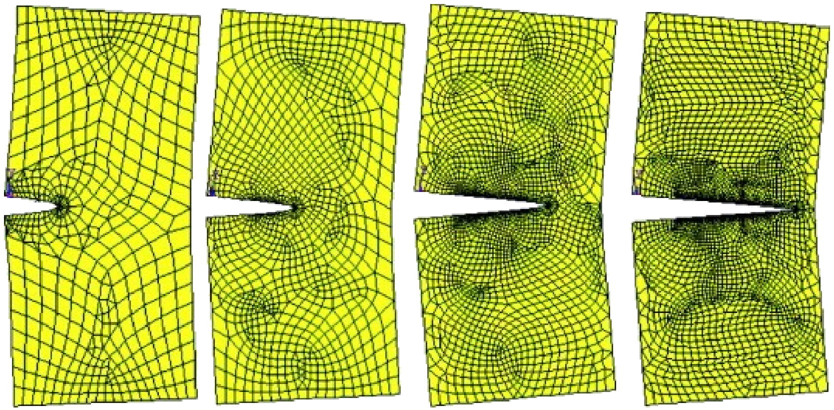
Accurate understanding of uncertainty in predictions

Allow organizations to share information but retain privacy of data

Explainable machine learning

Improved first principles simulations





Improved first principles quantum simulations leads to better inputs for machine learning to guide extrapolation of experimental data

Conclusion

Opportunity for predictive technologies in material sciences and pharmaceuticals

Apply quantum implementations of standard algorithms used in machine learning

Improve first principles calculations used to augment experimental data