Some building blocks for materials innovation

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Materials Science and Technology for Sustainable Development
Materials for efficient energy technology systems

Photovoltaic

Electricity

Excess electricity

Water splitting

H₂ fuel

Fuel cell
The economics of the great divergence

more complex technological systems, more productive nations
Materials complexity and technological progress

More building blocks (materials)...

...more complex technological systems
Studying nature’s building blocks to design new materials

\[ \sum \vec{F} = m\vec{a} \]

interacting electrons

\[ H(t)|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle \]

The Nobel Prize in Chemistry 1998

Photo from the Nobel Foundation archive.
Walter Kohn
Prize share: 1/2

Photo from the Nobel Foundation archive.
John A. Pople
Prize share: 1/2
Studying nature’s building blocks to design new materials

\[ \sum \vec{F} = m \vec{a} \]

...with neurons

\[ H(t) |\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle \]

jiggling atoms

interacting electrons

RESEARCH ARTICLE

MANY-BODY PHYSICS

Solving the quantum many-body problem with artificial neural networks

Giuseppe Carleo\(^1\) and Matthias Troyer\(^1,2\)

The challenge posed by the many-body problem in quantum physics originates from the difficulty of describing the nontrivial correlations encoded in the exponential complexity of the many-body wave function. Here we demonstrate that systematic machine learning of the wave function can reduce this complexity to a tractable computational form for some notable cases of physical interest. We introduce a variational representation of quantum states based on artificial neural networks with a variable number of hidden neurons. A reinforcement-learning scheme we demonstrate is capable of both finding the ground state and describing the unitary time evolution of complex interacting quantum systems. Our approach achieves high accuracy in describing prototypical interacting spins models in one and two dimensions.
Studying nature’s building blocks... with 0s and 1s
Graphene: a quantum material for energy and computing

two-layer graphene, with a twist
A ‘Legoland’ of 2D materials: Combinatorial explosion! 

graphene-like “building blocks”
Are we there yet?
The materials knowledge cycle
Towards autonomous labs for materials design
From complex network analysis to prototype Li-ion cells

Silicon-based Li-ion batteries

Battery tech startup Sila Nano lands $45 million and Tesla veteran Kurt Keity

2019, implementation

2014, calculation
Risk-sharing materials innovation

Academia

Triple helix model

Business

Public sector

building blocks for innovation and economic development

R & D

VENTURE CAPITAL

PRIVATE EQUITY

DEBT FINANCING

PROTOTYPE/PROOF OF CONCEPT

PILOT/DEMONSTRATION

COMMERCIALIZATION/MATURATION

MATURED/PRICE COMPETITION

TECHNOLOGICAL VALLEY OF DEATH

COMMERCIALIZATION VALLEY OF DEATH
Evidence-based RDI policy

knowledge creation in research networks: clusters (teams) as the elementary unit