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Artificial Intelligence for Intelligent Cities (Materials)

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Smart cities, smart materials

A Smart city is an urban setting that applies technology to enhance the benefits and diminish the shortcomings of urbanization for its citizens [1]”

Smart materials can sense, process, and respond to environmental stimuli without involving centralized resources [2]

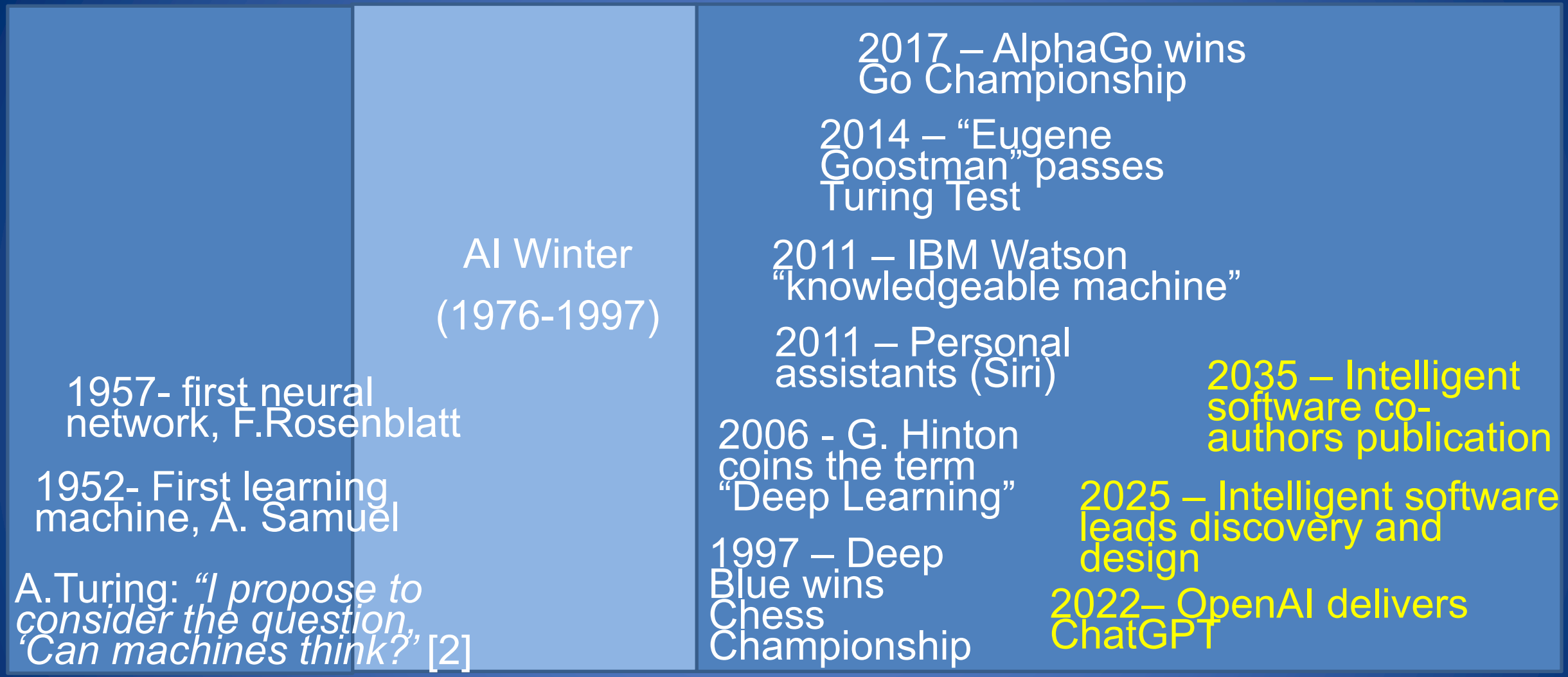
- Adaptive materials
- Self-healing materials
- “Living materials,” which may even use biological organisms
- Chemical machines for sensing and responding to environmental changes

[1] The Smart City Index
[2] R. Napolitano, W. Reinhart, and JP Gevaudan (2021) Science, 371 (2021) 1200

From “smart” to “intelligent”

Intelligent cities (materials) learn and respond to new challenges in real-time

A brief history of Artificial Intelligence [1]



[1] M. Stan, *Human and Artificial Intelligence* (2023)

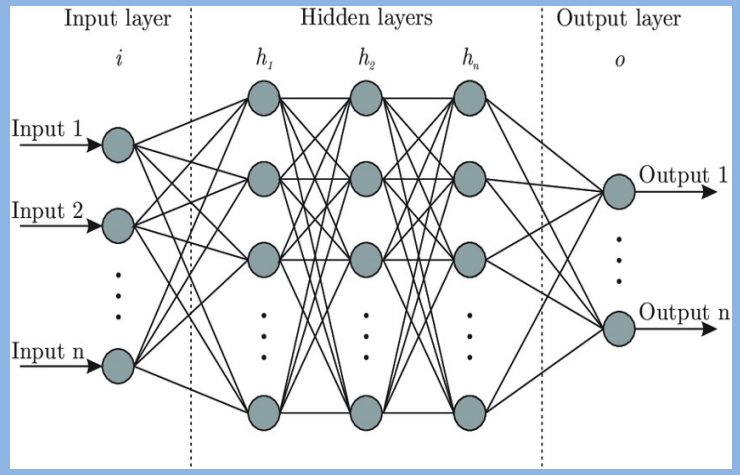
[2] Alan Turing, "Computing Machinery and Intelligence", 1950

AI components

Artificial Intelligence (AI): software that exhibits intelligence

Machine Learning (ML): AI algorithms that learn from data and improve

Deep Learning: ML algorithms based on neural networks



Computer vision

Robotics

Natural Language Processing

M. Stan, *Human and Artificial Intelligence* (2023)

AI for improved computers

Hafnium dioxide (hafnia) HfO_2

Introduced by Intel in 2007 as a replacement for silicon oxide in field-effect transistors (FET)

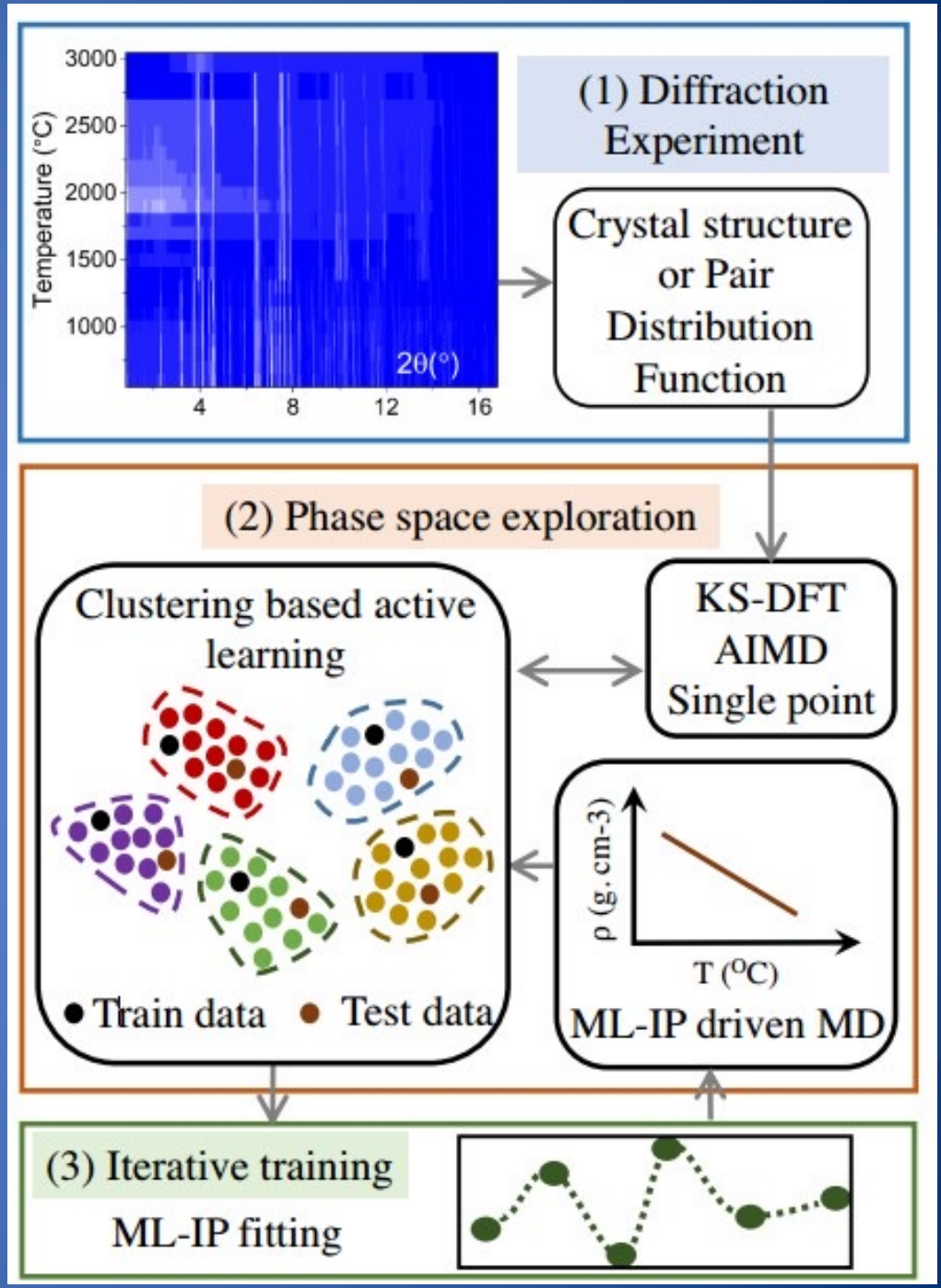
Used in dynamic random-access memory (DRAM) to increase the capacity of computer memory and make the computers faster

Methodology

(1) HfO_2 samples are acoustically levitated, then x-ray and neutron diffraction measurements initialize the AI-driven molecular dynamics calculations of atomic structures

(2) A deep-learning algorithm explores the phase space, screening for best atom configurations

(3) AI learns from experiments and simulations, re-trains the model, and makes better predictions



Results

- AI learns from experiments and finds the optimal inter-atomic potential and crystal structure
- The method reduces human time and effort by a factor of 10 while maintaining accuracy (compared to DFT)
- The resulting computer memory has more capacity and is way faster

G. Sivaraman, M. Stan *et al*. Phys. Rev. Let. 126 (2021) 156002
G. Sivaraman, M. Stan *et al*. npj-Comp. Mater, 4 (2020) 104

AI for improved batteries

Conventional Li-ion batteries:

- Limited energy density due to graphite anode
- Large volume change at certain Li content leading to collapse of the cathode
- Risk of thermal runaway

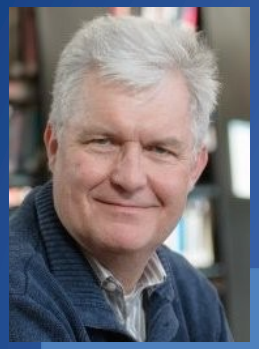
Solid-state batteries:

- Higher energy density due to compatibility with Li metal anode
- Dramatically improved safety

RSC Advances 2018, 8, 40172-40186

Methodology and team

John Low



Hakim Iddir

Noah Paulson

Initial AIMD

LAMMPS

ML Training

Predict with UQ

Active selection

Improved cathode

Juan Garcia

Joshua Gabriel

Marius Stan

Quantum Optimization

DeepMD-kit

VASP

J. Garcia, M. Stan et. al, J. Phys. Chem. C, 125 (2021) 27130.

Results

- The machine learning software predicted the collapse of a Li ion NMC-111 ($Li_{1.05}Ni_{0.33}Mn_{0.33}Co_{0.33}O_2$) cathode at an amount of 0.2 Li at room temperature

- The machine learning software provided an acceleration of 10x, while maintaining accuracy, with respect to the underlying training data derived from DFT calculations

Recent AI applications for smart cities

A self-driving c
of Las Vegas [

A swarm of AI drones can autonomously evaluate fire and conflict situations [Andy Dean photography/Shutterstock.com]

ous delivery system at
ity of Arizona [M. Stan]

Human and Artificial Intelligence

	Pros	Cons
Human Intelligence	• Common sense • Critical Thinking • Intuition • Creativity • Sense of humor	• Unreliable • Slow • Limited processing capacity • Impacted by mood • Requires extended rest, recovery
Artificial Intelligence	• Fast response • Can quickly process large data sets and streams • Powerful, reliable memory • Available most of the time	• No creativity • No personality • Can increase unemployment • Can deteriorate human abilities • Might take over human society

"I view it as a big responsibility to get it right … I think we'll be able to do these things better over time." Sundar Pichai (Google)

"We have a five to ten percent chance of success of creating safe AI." Elon Musk (Tesla)

M. Stan, *Human and Artificial Intelligence* (2023)

Some things to consider

- Intelligent Cities (Materials) learn and respond to new challenges in real-time
- Teams of humans and AI have created improved materials for computer memory and battery cathodes for autonomous devices in smart cities
- By 2035 intelligent software will co-author scientific articles
- AI has many benefits; the main danger is the people who use it
- Legal AI frameworks are best developed by politicians, technologists and AI
- Romania has the brain power to create intelligent cities. But it needs …