

# **Physical systems for thermodynamic computing (Some examples)**



**J. Joshua Yang**

The Department of Electrical and Computer Engineering  
University of Massachusetts, Amherst

# outline

**1. Memristor introduction**

**2. Simple computing without thermodynamics  
(supervised learning)**

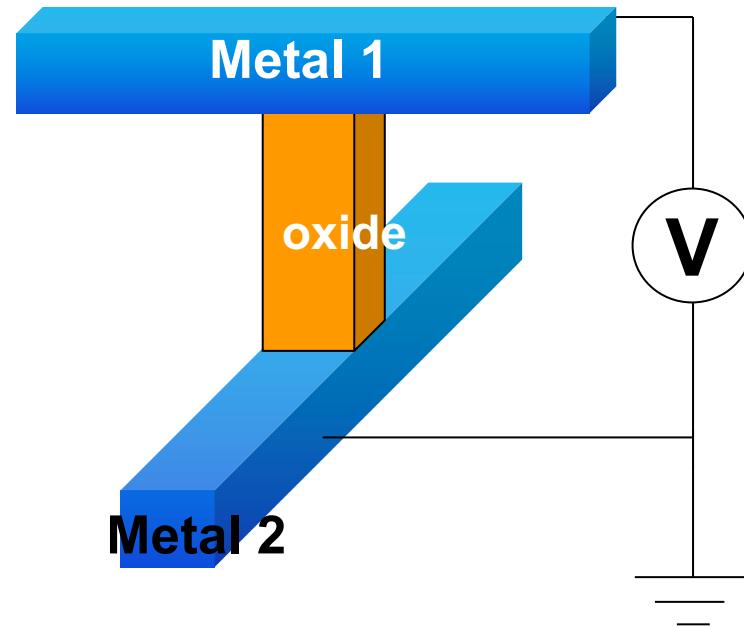
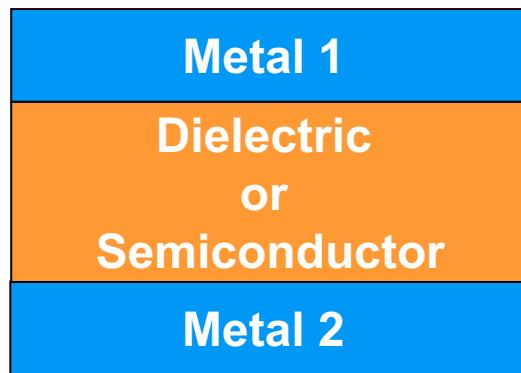
**3. Advanced computing with thermodynamics  
(unsupervised learning)**

**4. Other physical systems**

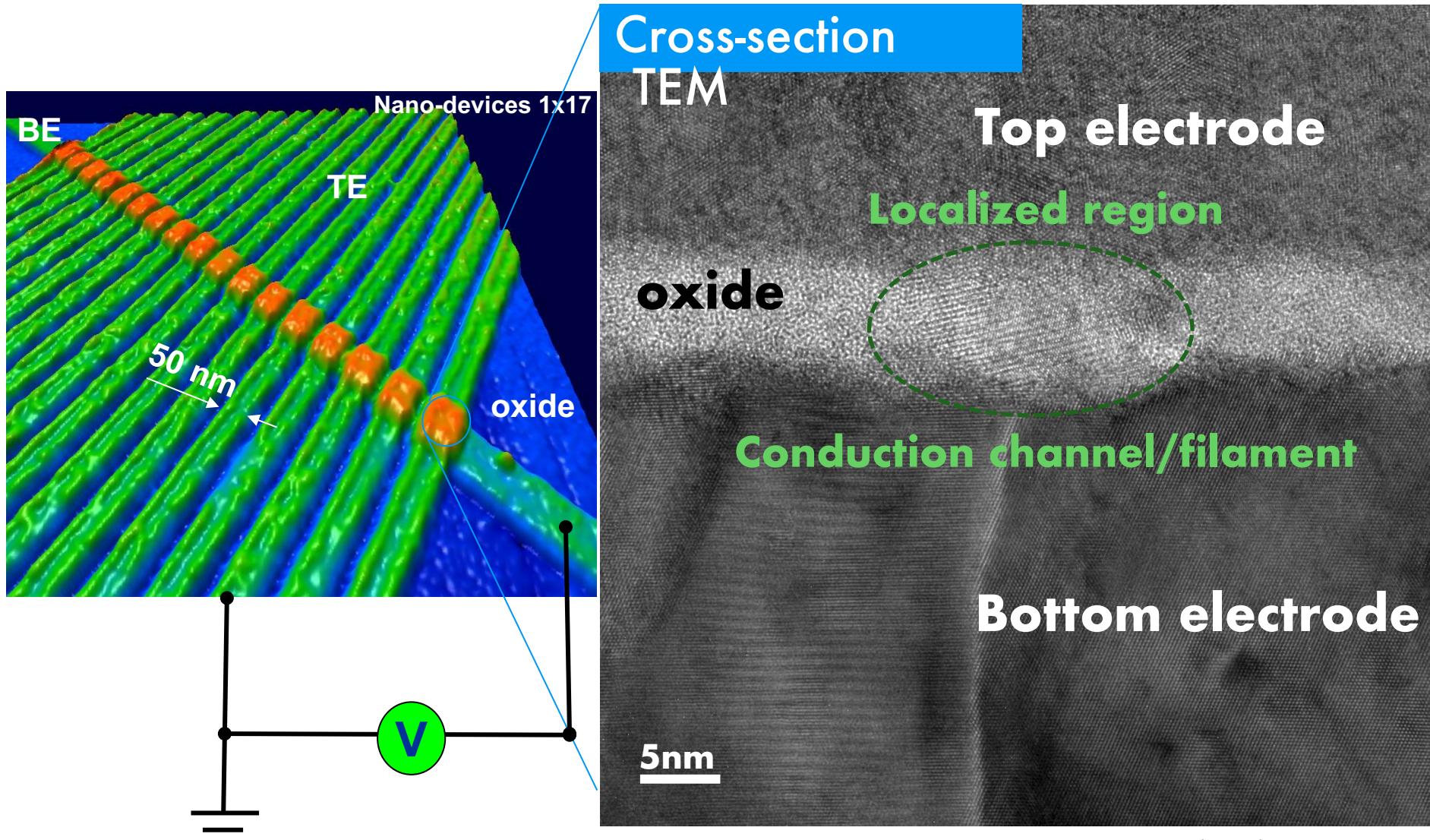
# Memristor introduction

# Simple but complicated materials and device

Complicated physics, chemistry, materials, i.e., thermodynamics, issues

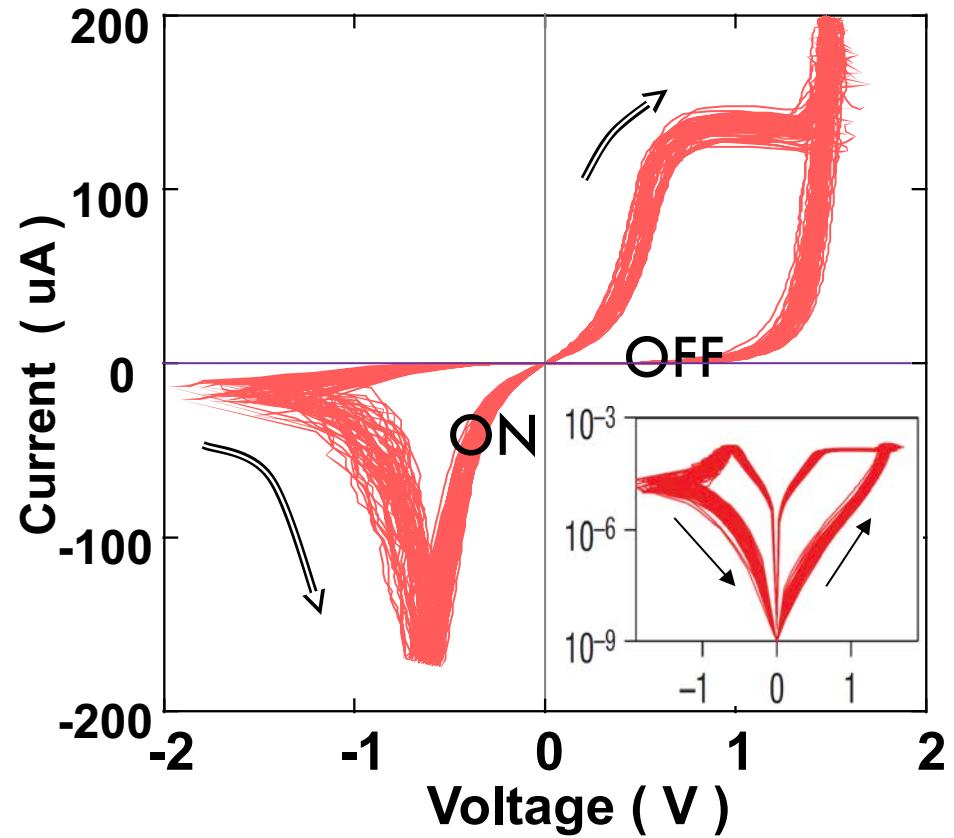
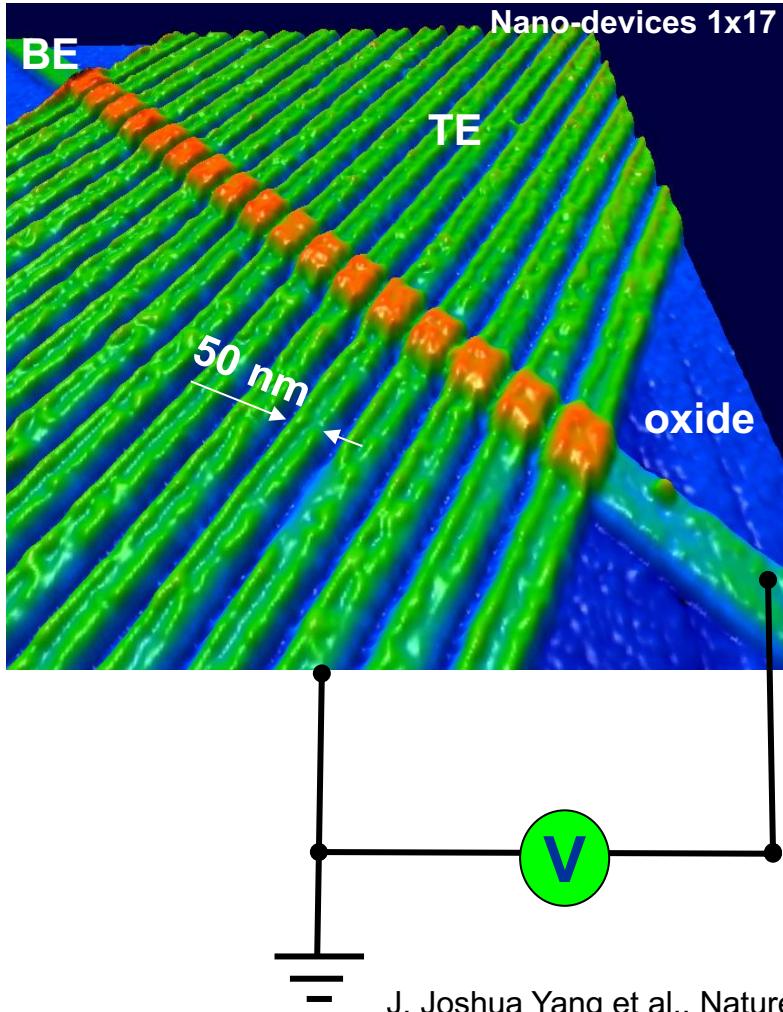


# The first oxide nanodevice



J. Joshua Yang et al., Nature Nanotechnology 3, 429 (2008)

# The signature of memristive devices



J. Joshua Yang et al., Nature Nanotechnol. 3, 429 (2008)

# Promises and Challenges

## Promises

1. *Speed (85ps)*
2. *Scalability (2nm)*
3. *Multilevel (>64)*
4. *Stackability (>8 layers)*
5. *CMOS compatibility*
6. *Non-volatility (>10years)*
7. *Non-destructive reading*
8. *Low cost*
9. .....

## Challenges

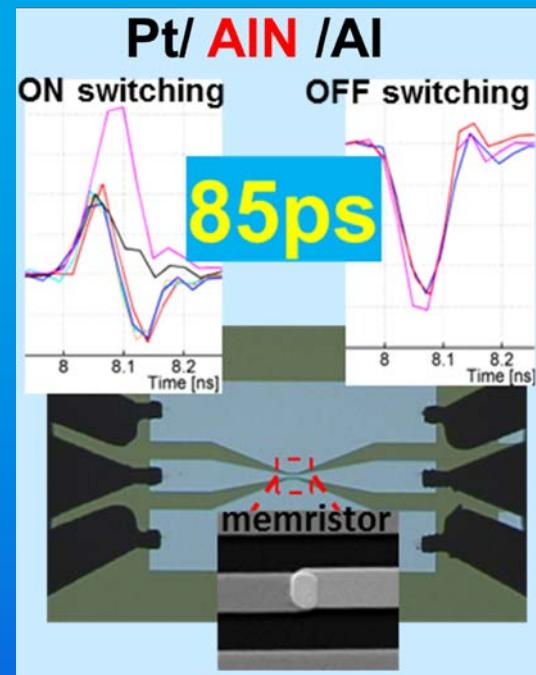
- *Mechanism*
- *Access device in large array*  
*(Transistor, selector)*
- *Desirable dynamics*  
*(Diffusive memristor)*

# Promises

## Promises

1. Speed (85ps)
2. Scalability (2nm)
3. Multilevel (>64)
4. Stackability (>8 layers)
5. CMOS compatibility
6. Non-volatility (>10years)
7. Non-destructive reading
8. Low cost
9. .....

85ps ON/OFF switching



B. J. Choi, et al, *Adv. Funct. Mater.* 26, 5290, (2016).

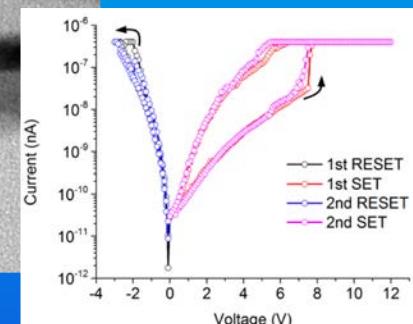
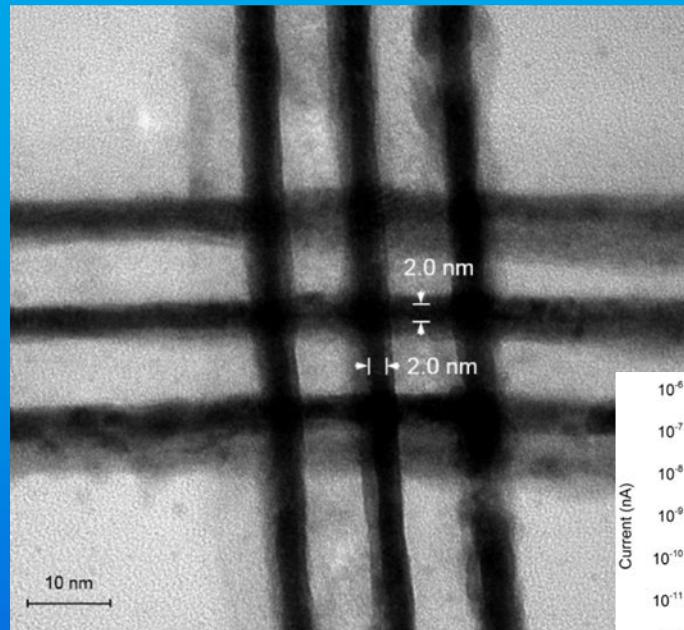
T., Antonio C., John Paul Strachan, G. Medeiros-Ribeiro, and R. Stanley Williams.  
"Sub-nanosecond switching of a tantalum oxide memristor." *Nanotechnology* 22, no. 48 (2011): 485203.

# Promises

## Promises

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9. .....

## 2nm x 2nm memristor crossbar



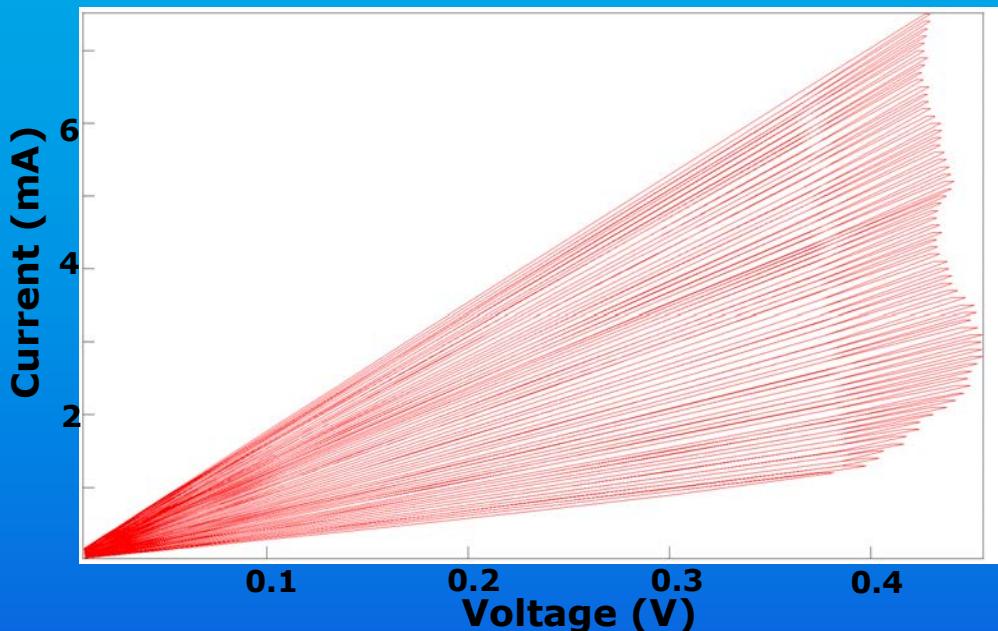
S. Pi et al., *Nature Nanotechnology* **14**, 35 (2018).  
(Q. Xia)

# Promises

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9. .....

**64 resistance levels**



N. Ge et al., unpublished (2018).

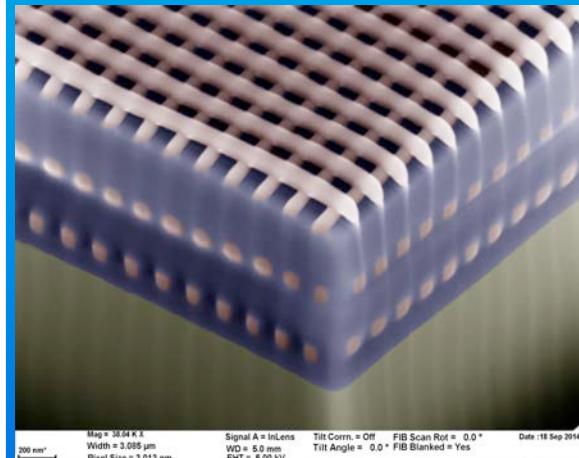
# Promises

## Promises

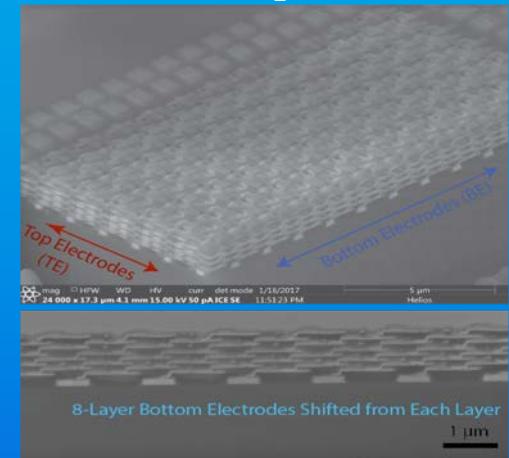
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8. ***Low cost***
9. .....

## 3D integration of memristor on CMOS

5 Layers



8 Layers



C. Li et al., Nature Comm.  
8, 15666 (2017)  
(Q. Xia)

P. Lin et al., under review  
(2018)  
(Q. Xia)

# Promises and Challenges

## Promises

1. ***Speed (85ps)***
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## Challenges

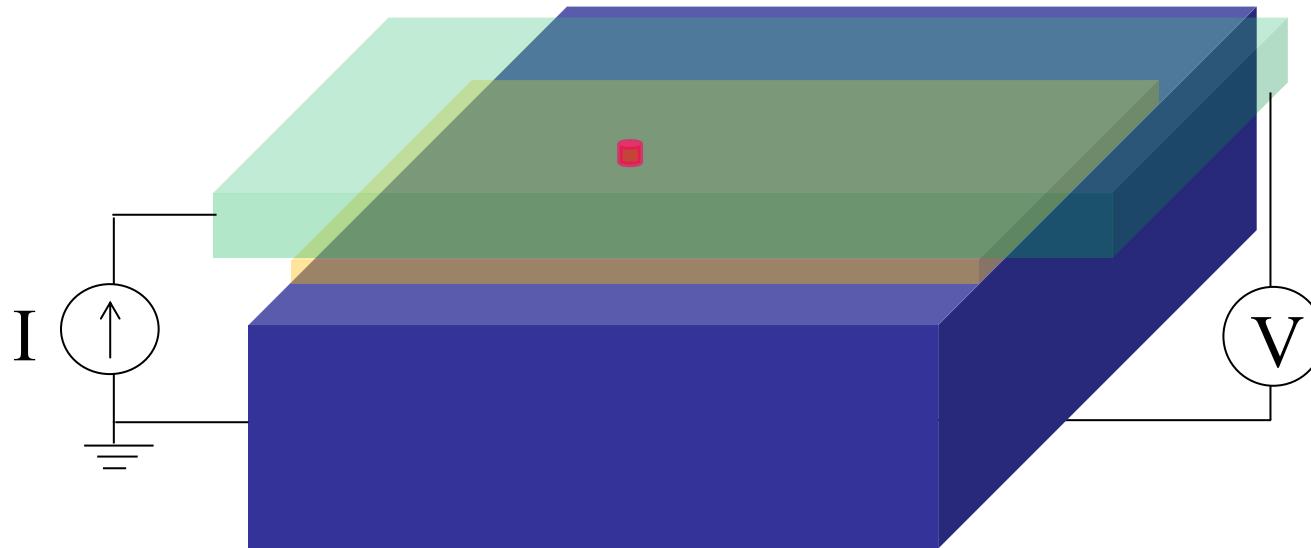
(priority of research directions at device level)

- **Mechanism**
- ***Access device in large array  
(Transistor, selector)***
- ***Desirable dynamics  
(Diffusive memristor)***

# Difficulty in understanding the mechanism

**Whatever changes is:**

- Buried under the top electrode (invisible)
- Localized both laterally and vertically (very small:  $1 \sim 100\text{nm}$ )
- Random location (elusive)
- Take place very fast ( $\sim 0.1\text{ns}$ )



# A simplified Mechanism in a model system: TiO<sub>x</sub> devices

**Where:**

Bulk (oxide only) or interface (oxide/electrode)?

**What:**

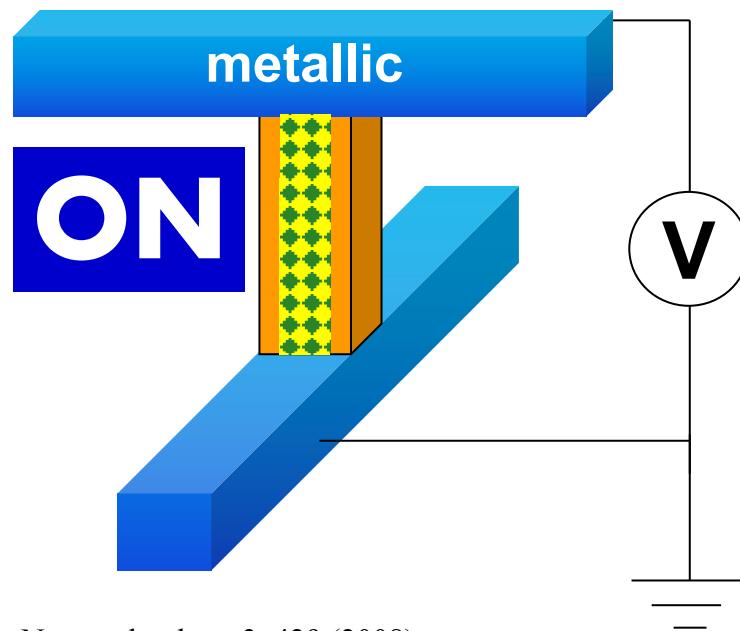
Active species ( $V_o^{2+}$ ) responsible for the switching?

**How :**

localized switching channel grows (ON) and retracts (OFF)

There are other types of mobile ions  
e.g. Ag:SiN<sub>y</sub>O<sub>x</sub>

Diffusive memristor

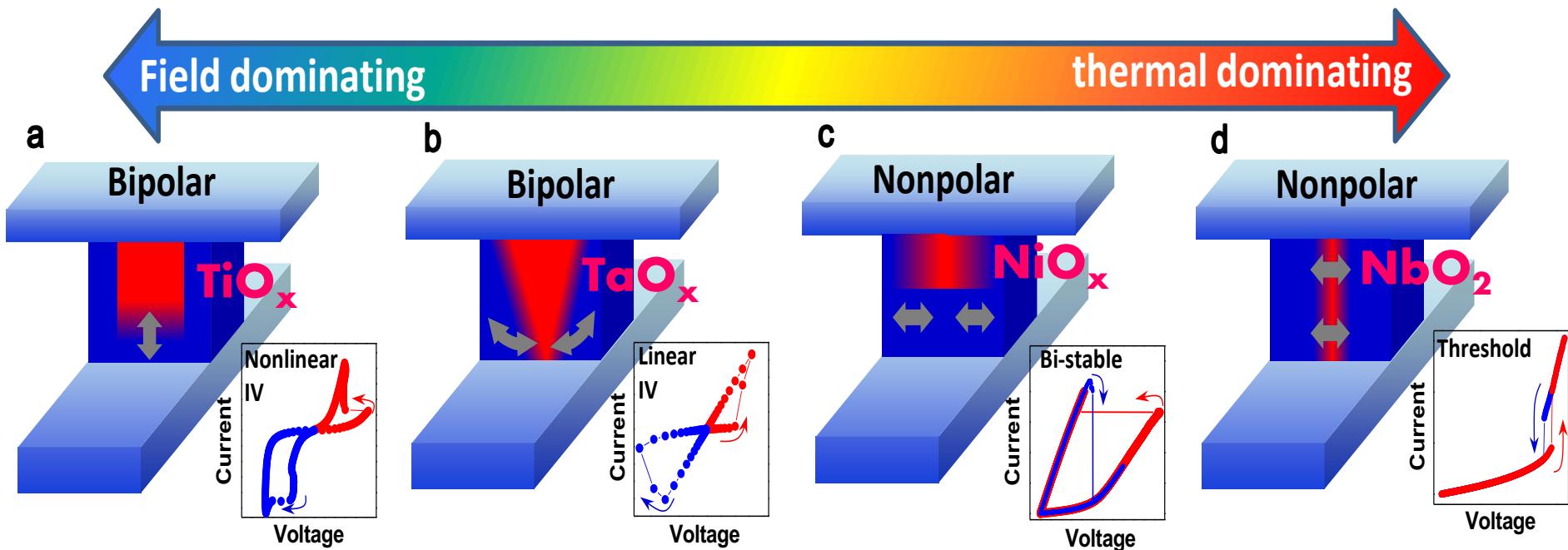


J. Joshua Yang et al., Nature Nanotechnology 3, 429 (2008)

J. Joshua Yang et al., Advanced Materials, 21, 3754 (2009)

# Mechanisms: Driving forces and switching types

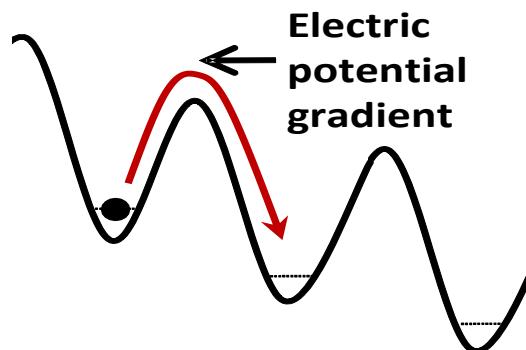
Switching is a result of **ionic motion** under the combined effect of **electric field and Joule heating**



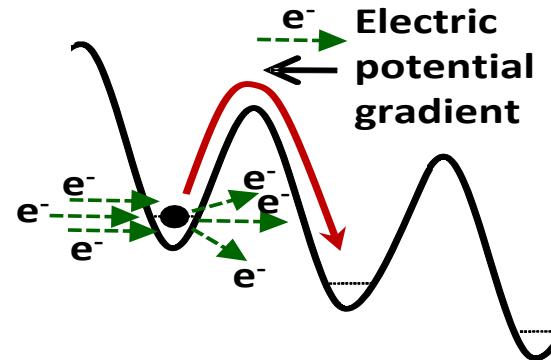
J. Joshua Yang et al., Nature Nanotechnology 8, 13 (2013)

# Mechanisms: Ionic transport mechanisms

**drift**

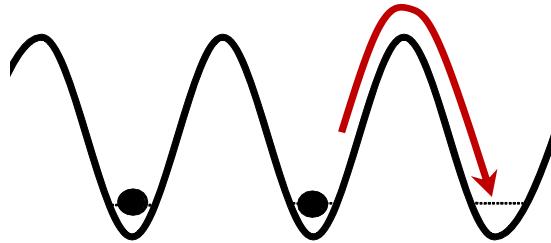


**Electromigration**



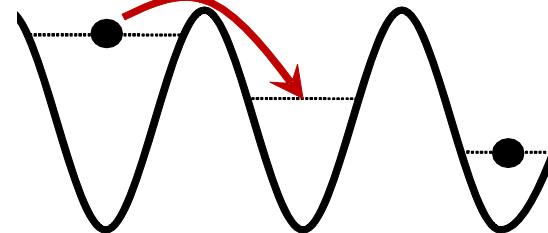
**Fick Diffusion**

→ Concentration gradient



**Thermophoresis**

← Temperature gradient



J. Joshua Yang et al., Nature Nanotechnology **8**, 13 (2013)

# Promises and Challenges

## Promises

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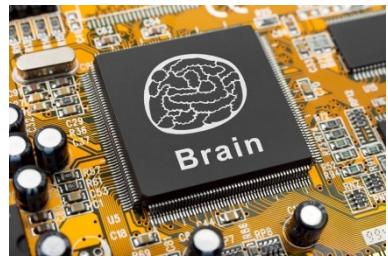
## Challenges

(priority of research directions at device level)

- ***Mechanism***
- ***Access device in large array  
(Transistor, selector)***
- ***Desirable dynamics  
(Diffusive memristor)***

# Simple computing without thermodynamics

# Computing with memristive devices at UMass



Source: Institute of  
Neuroinformatics (INI)

New  
building  
blocks

Artificial  
Synapse

*Nature Materials* **16**, 101 (2017).  
*Nature Comm.* **8**, 752 (2017).

Artificial  
Neuron

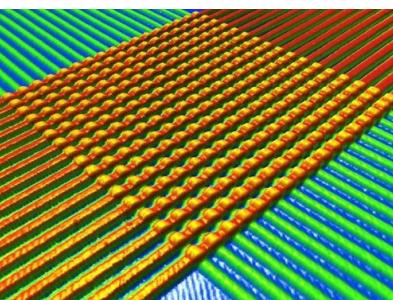
*Nature Electronics*, **1**, 137 (2018).  
*Nature Comm.* **9**, 417 (2018).  
*Nature Comm.* **9**, 3208 (2018).

Memristor

Dot Product  
Engine

Accelerate  
Deep Neural  
Network

*Nature Electronics* **1**, 52 (2018).  
*Adv. Mater.* **29**, 1705914 (2018).  
*Nature Communications* **9**, 2385 (2018).  
*Nature Machine Intelligence* **1**, Accepted (LSTM, 2018)



Source: HP Lab

Novel  
Ultra  
Large  
Array  
Operation  
Other applications  
(some dynamics)

Memory,  
Robotics,  
Security...

*Nature Materials* **16**, 396 (2017). *Nature Electronics* **1**, 130 (2018).  
*Nature Comm.* **8**, 882 (2017). *Adv. Func. Mater.* **27**, 1704862 (2017).  
*Nature Comm.* **8**, 15666 (2017). *Adv. Mater.* **29**, 1604457 (2017).  
*Nature Electronics* **1**, 548 (2018).

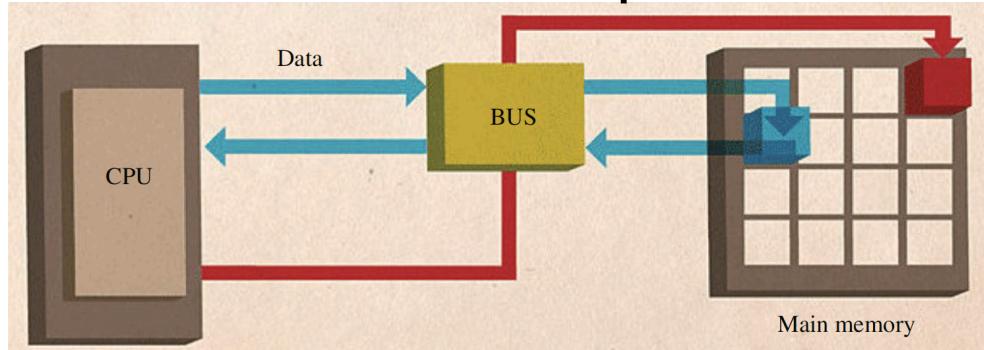


Source:  
<http://www.google.com/selfdrivingcar/>

Traditional AI approaches  
(little dynamics)

# Issues with classical computer hardware in big-data era

## Classical computer



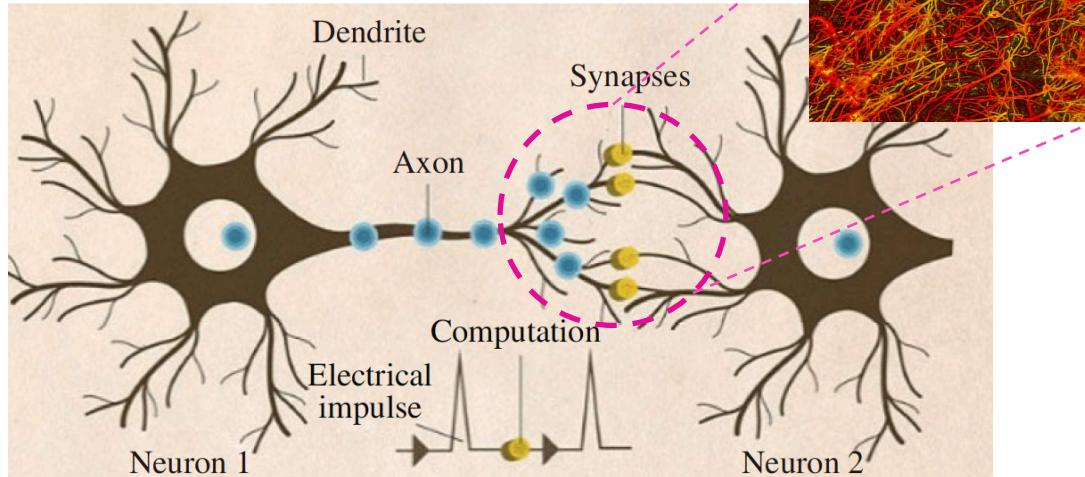
## Devices:

reaching physical limit for scaling down (Moore's law is over)

## Architecture:

- separate processor and storage (Von Neumann bottleneck)
- Sequential process
- Analog/Digital conversion

## Brain networks



## In Brain:

Neurons, Synapses and networks

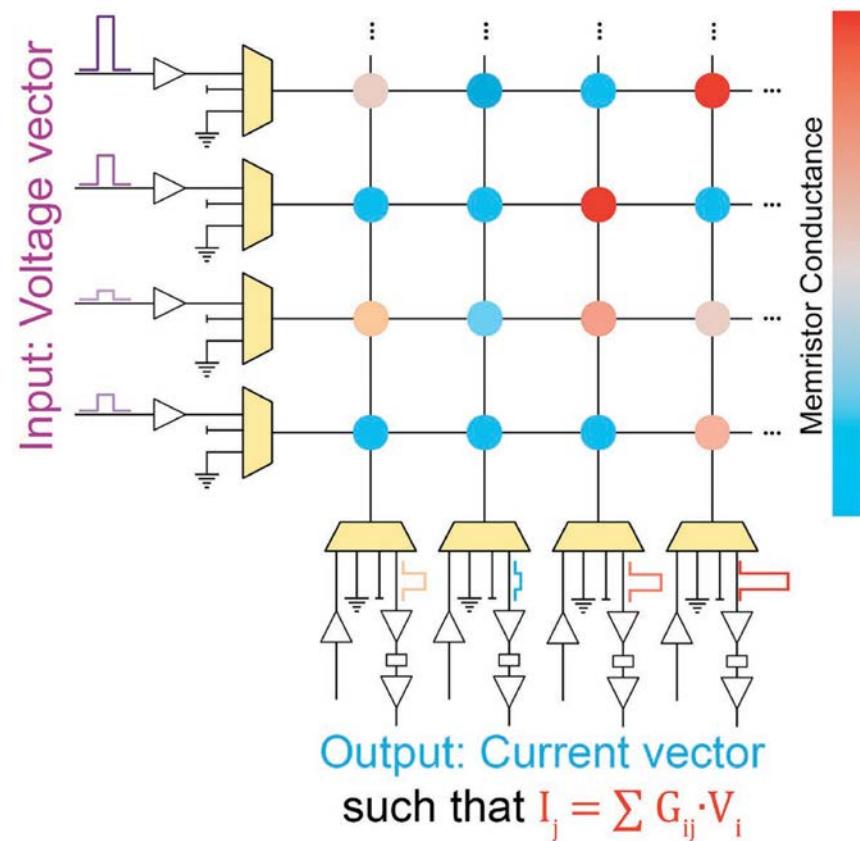
- In-memory computing
- Parallel computing (instead of sequential)
- Analog computing

U., Navnidhi, S. Joshi, J. Joshua Yang. "Synaptic electronics and neuromorphic computing." *Science China Information Sciences* 59, 061404 (2016)

# Physical computing application: Dot-product Engine (for Deep Neural Network)

- **Vector x Matrix** multiplications
- Computation intensive tasks  
(many multiplication and addition steps)

Only one step in dot-product engine

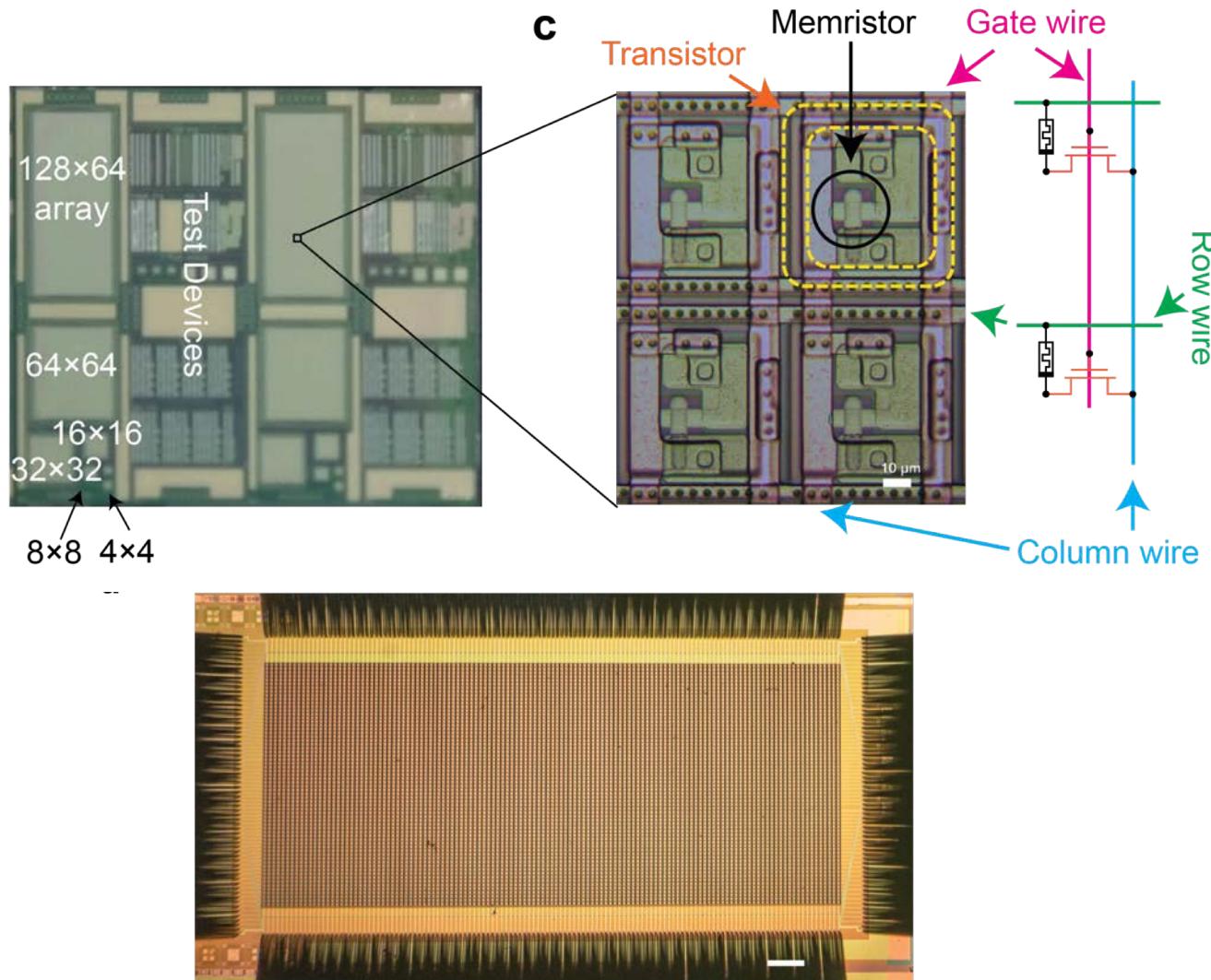


With **orders of magnitude**  
**Improvement in**  
**speed and power efficiency!**

"Dot-Product Engine for Neuromorphic Computing: Programming 1T1M Crossbar to Accelerate Vector-Matrix Multiplication", *the 53rd Design Automation Conference (DAC), 2016.*

*M. Hu et al., Adv. Mater. 29, 1705914 (2018).*

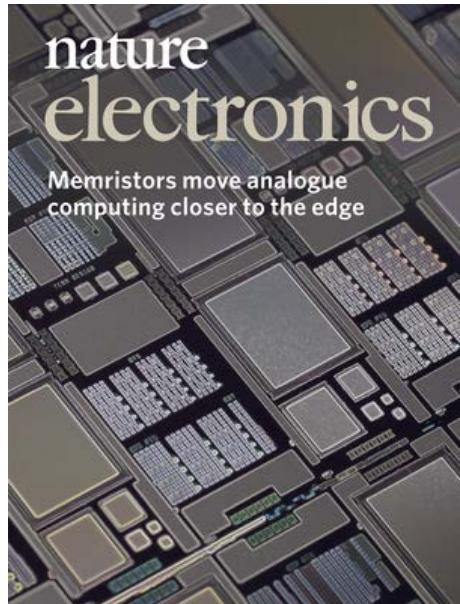
# Deep Neural Network: Dot-Product Engine (DPE)



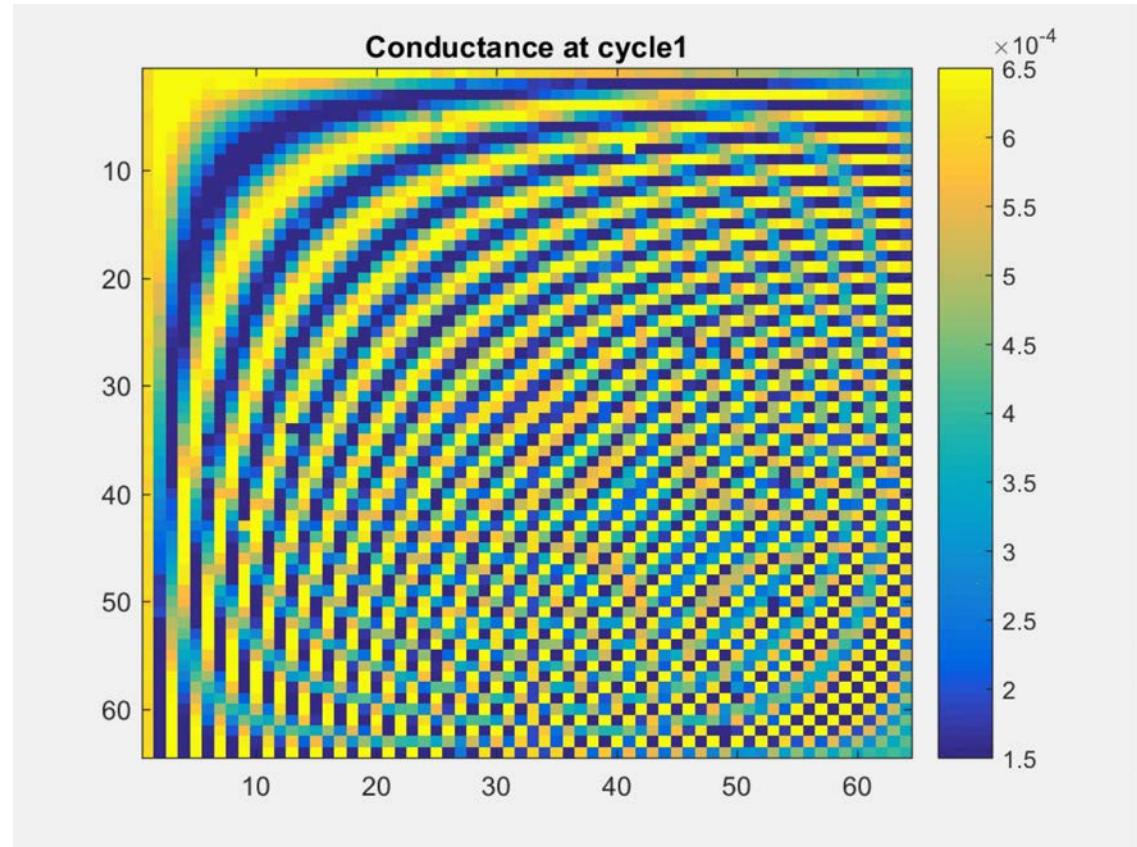
C. Li et al, Nature Electronics 1, 52 (2018)

(collaborated with Stan Williams & John Paul Strachan)

# Accurate programming of resistance states in the array



(Cover article of inaugural issue)



C. Li et al., Nature Electronics 1, 52 (2018)

# Image Processing (experimental demo)

## Image Compression Using Analog Memristor Array (DCT) (20:3 compression ratio)

Original image



Software processed



Memristor array processed (Experimental)



C. Li et al., Nature Electronics 1, 52 (2018)

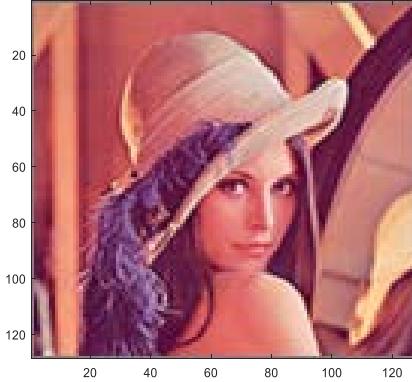
# Image filtering (experimental demo)

7 Different Filters Applied at the Same Time

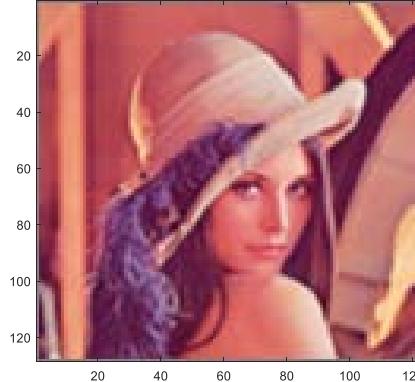
Original



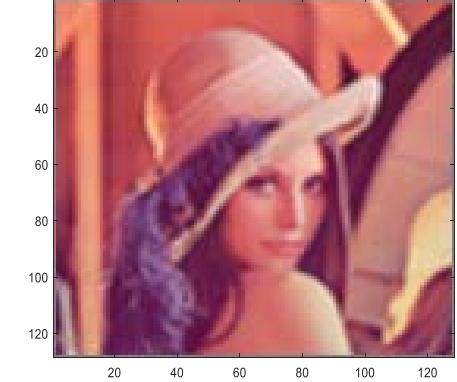
Gaussian



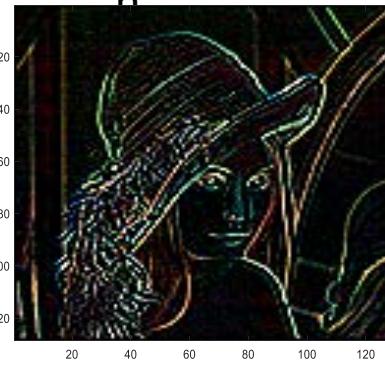
Disk



Average



Laplacia



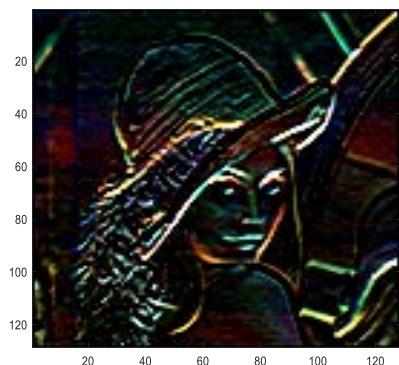
LoG



Prewitt (Horizontal)



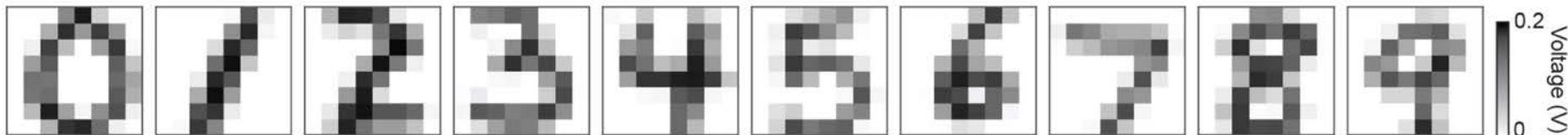
Sobel (Horizontal)



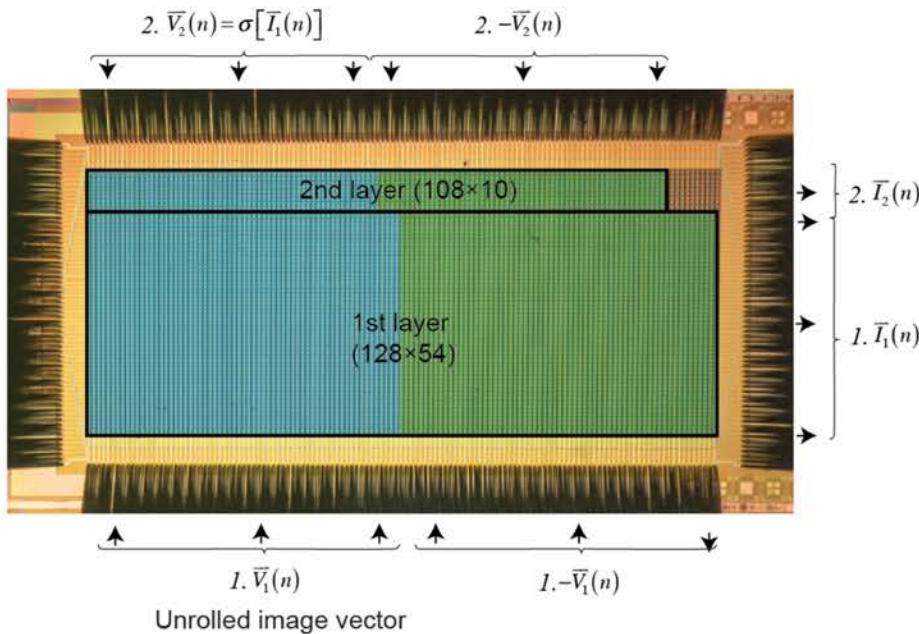
C. Li et al., Nature Electronics 1, 52 (2018)

# 2-layer Neural Network with supervised learning

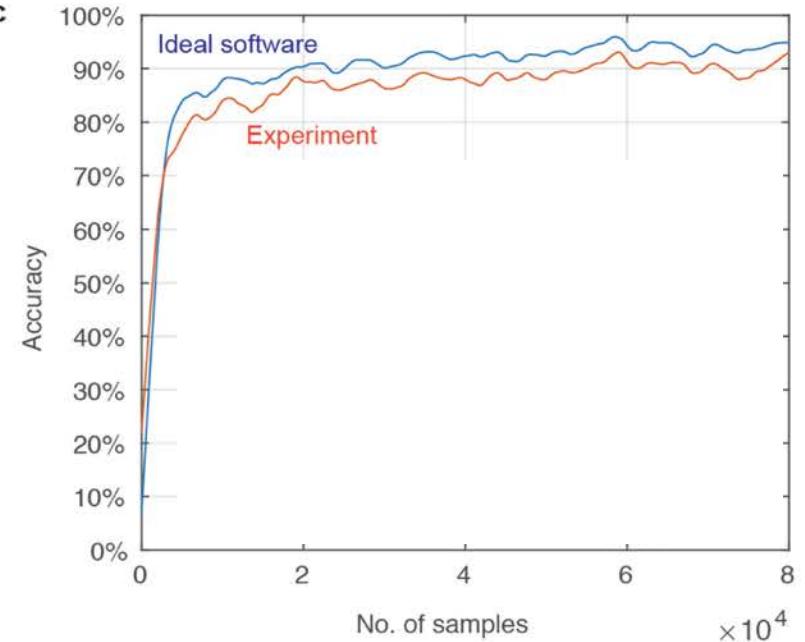
a MNIST grayscale image cropped & downsampled to 8×8



b



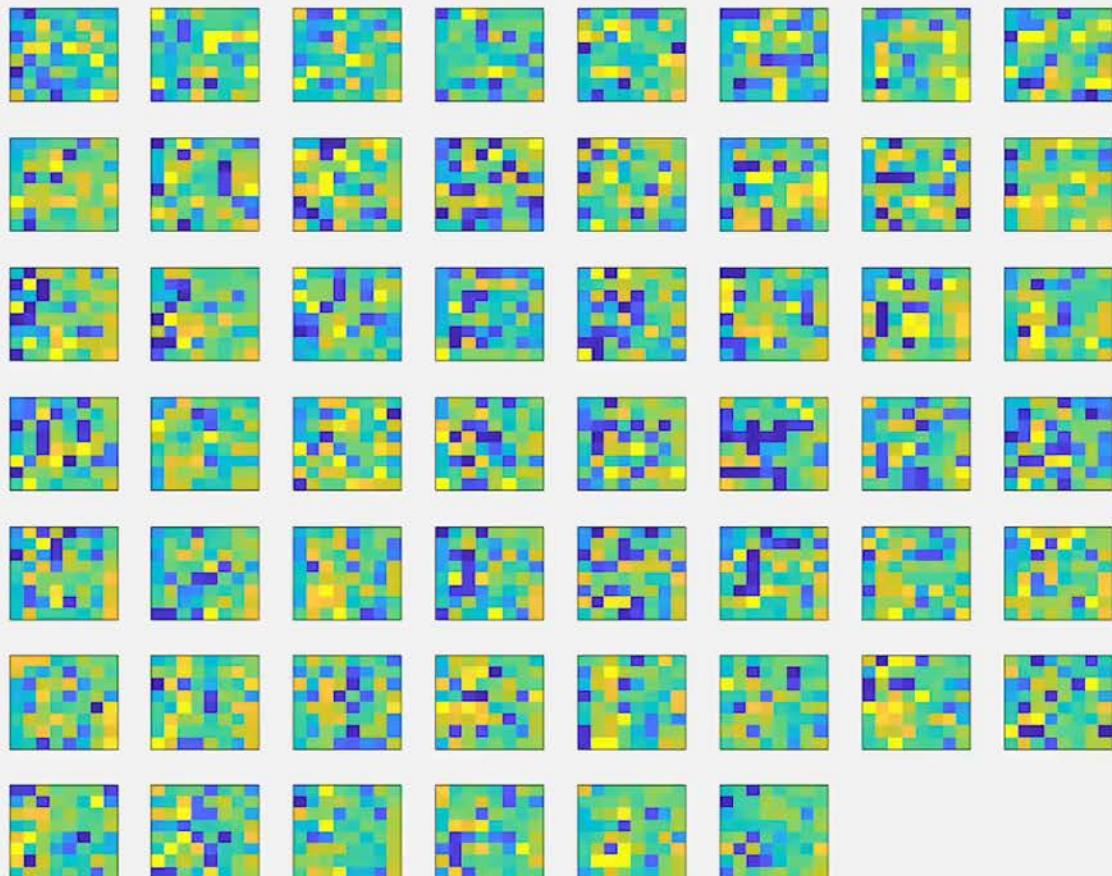
c



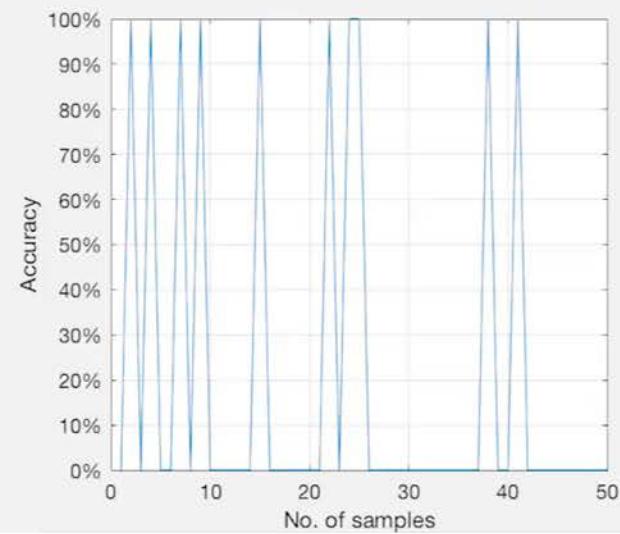
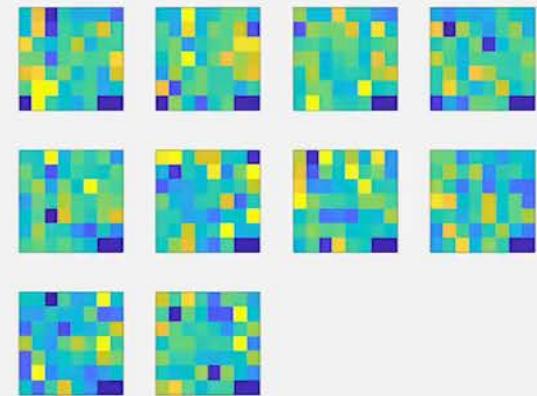
Li et al., Nature Communications 9, 2385 (2018).

# 2-layer Neural Network with supervised learning

1st layer weights



2nd layer weights



Li et al., Nature Communications 9, 2385 (2018).

# **More advanced computing (with thermodynamics)**

# Computing with memristive devices at UMass



Source: Institute of  
Neuroinformatics (INI)

New  
building  
blocks

Artificial  
Synapse

*Nature Materials* **16**, 101 (2017).  
*Nature Comm.* **8**, 752 (2017).



Source:  
<http://www.google.com/selfdrivingcar/>

Bio-inspired approach  
(important thermodynamics)

Artificial  
Neuron

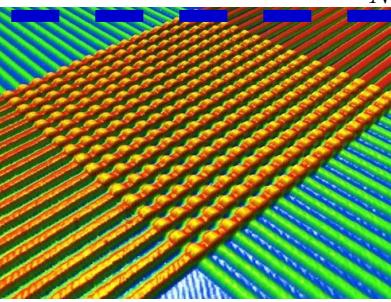
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Dot Product  
Engine

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*Nature Communications* **9**, 2385 (2018)  
*Nature Machine Intelligence* **1**, Accepted (LSTM, 2018)

Accelerate  
Deep Neural  
Network



Source: HP Lab

Novel  
Ultra  
Large  
Array

Operation

Other applications  
(some dynamics)

Memory,  
Robotics,  
Security...

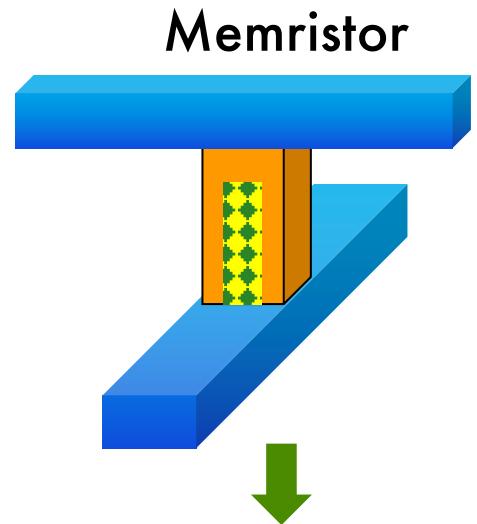
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Traditional AI approaches  
(little dynamics)

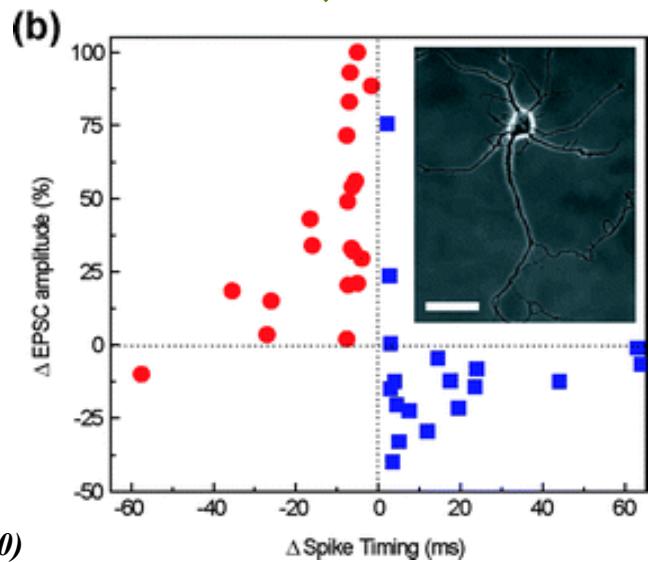
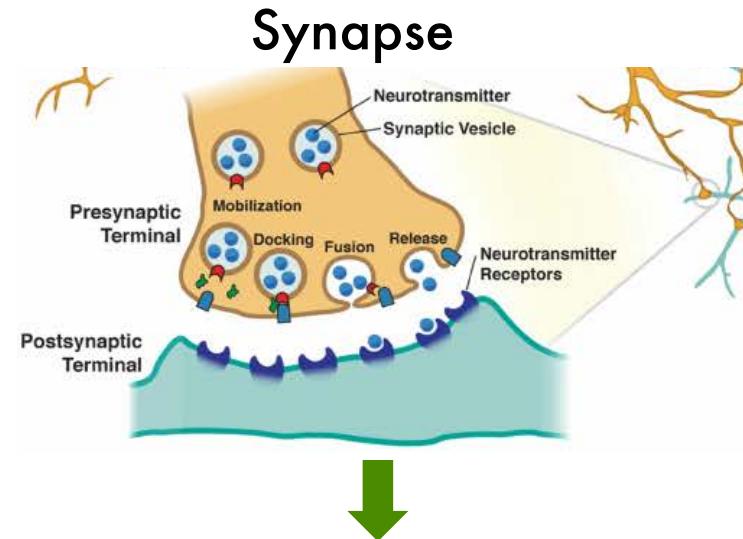
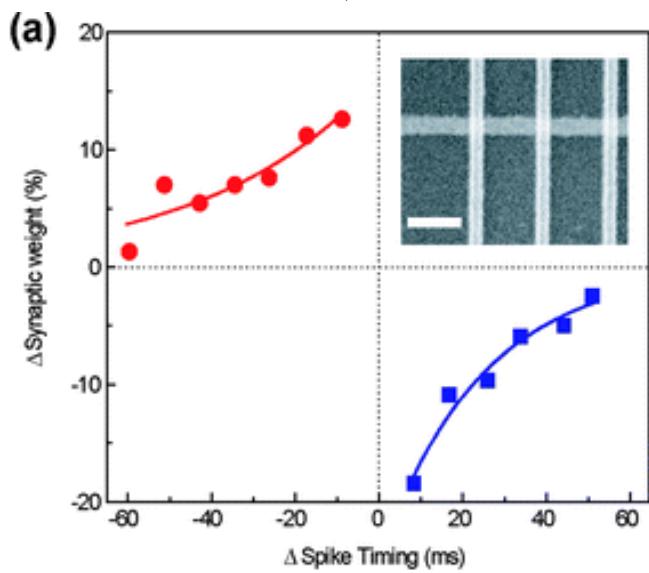
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*Adv. Func. Mater.* **27**, 1704862 (2017).  
*Adv. Mater.* **29**, 1604457 (2017).

# Problems with traditional memristors for synapse: lack of synaptic dynamics

## Spike-timing dependent plasticity (STDP)

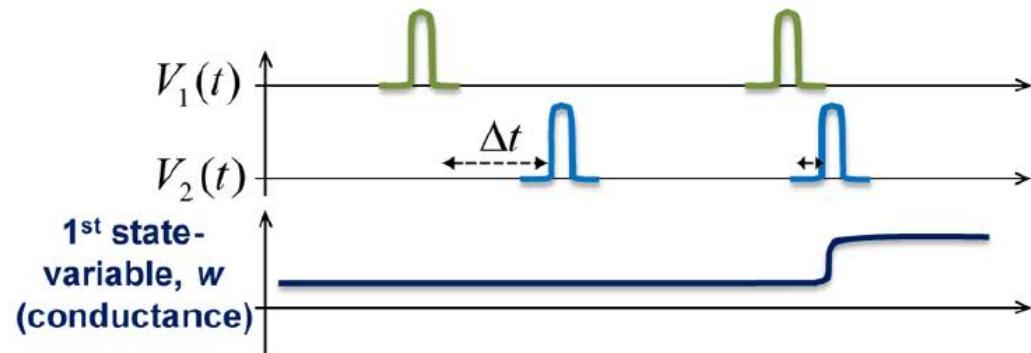
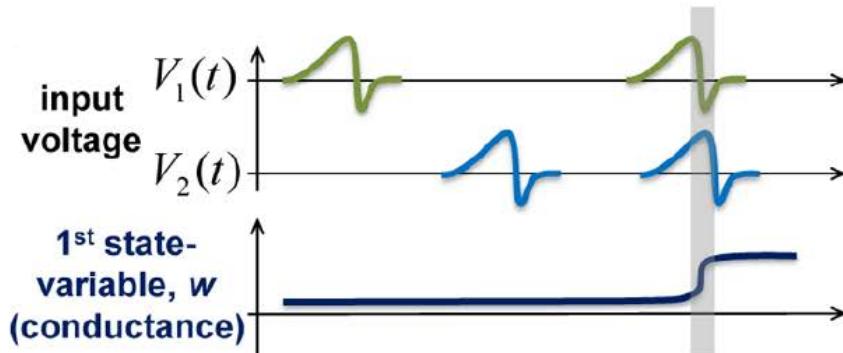


Indirect STDP



*Nano Lett. 10, 1297 (2010)*

# Synapse: spike timing carries the information!



(Umich) Nano Lett. 15, 2203 (2015), Adv. Funct. Mater. 25, 4290 (2015)

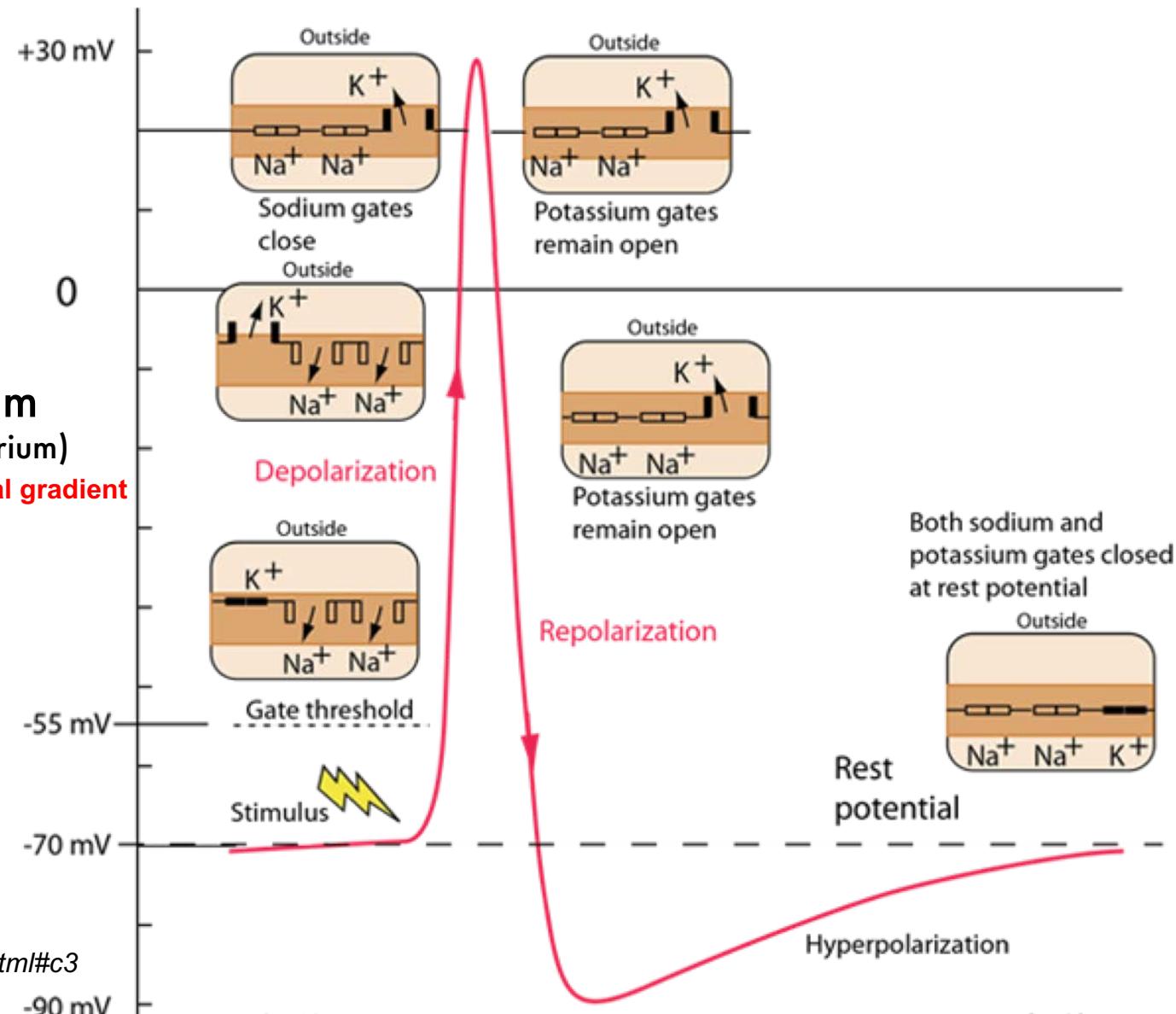
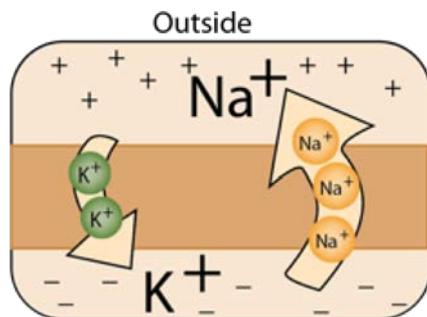
- Higher energy (not sparse spikes)
- More complicated circuits and algorithms
- Only phenomenological emulation of one or two functions and missing most others

- Dynamics is critical for synaptic functions
- With dynamics, many synaptic functions come out naturally and simultaneously!!

**Amplitude is less important, timing carries the information → synaptic dynamics!**

# Thermodynamics in neuronal computing: action potential

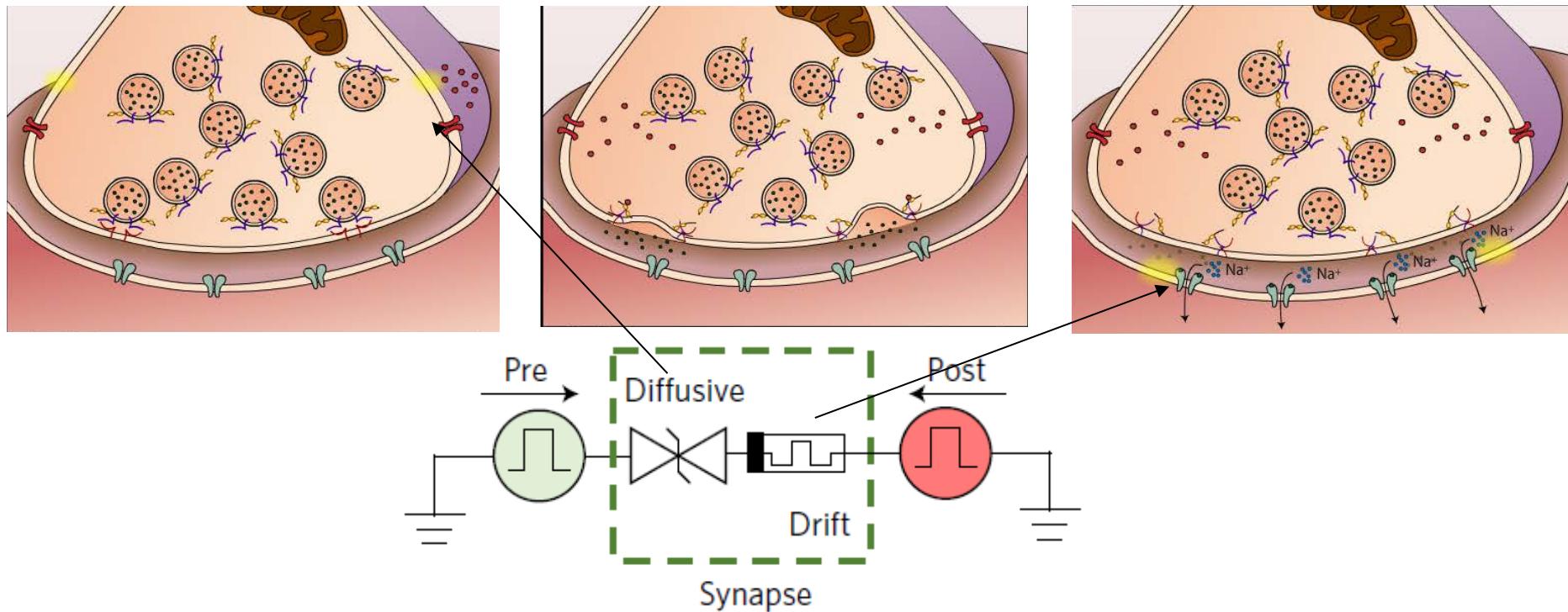
ATP pump to keep neuron in equilibrium  
(out of thermodynamic equilibrium)  
Energy is stored in electrochemical gradient



<http://hyperphysics.phy-astr.gsu.edu/hbase/Biology/actpot.html#c3>

# Reading process: similar role of Ca and Ag

Impulse from upper axon terminal → if large enough, it opens the voltage-controlled calcium channels in pre-neuron, Ca diffuses through →neurotransmitter release → open receptors in post-neuron → ions like  $\text{Na}^+$  go into post-neuron, generating impulse, passing on. The postsynaptic response (impulse) is weighted by for example the number of receptors

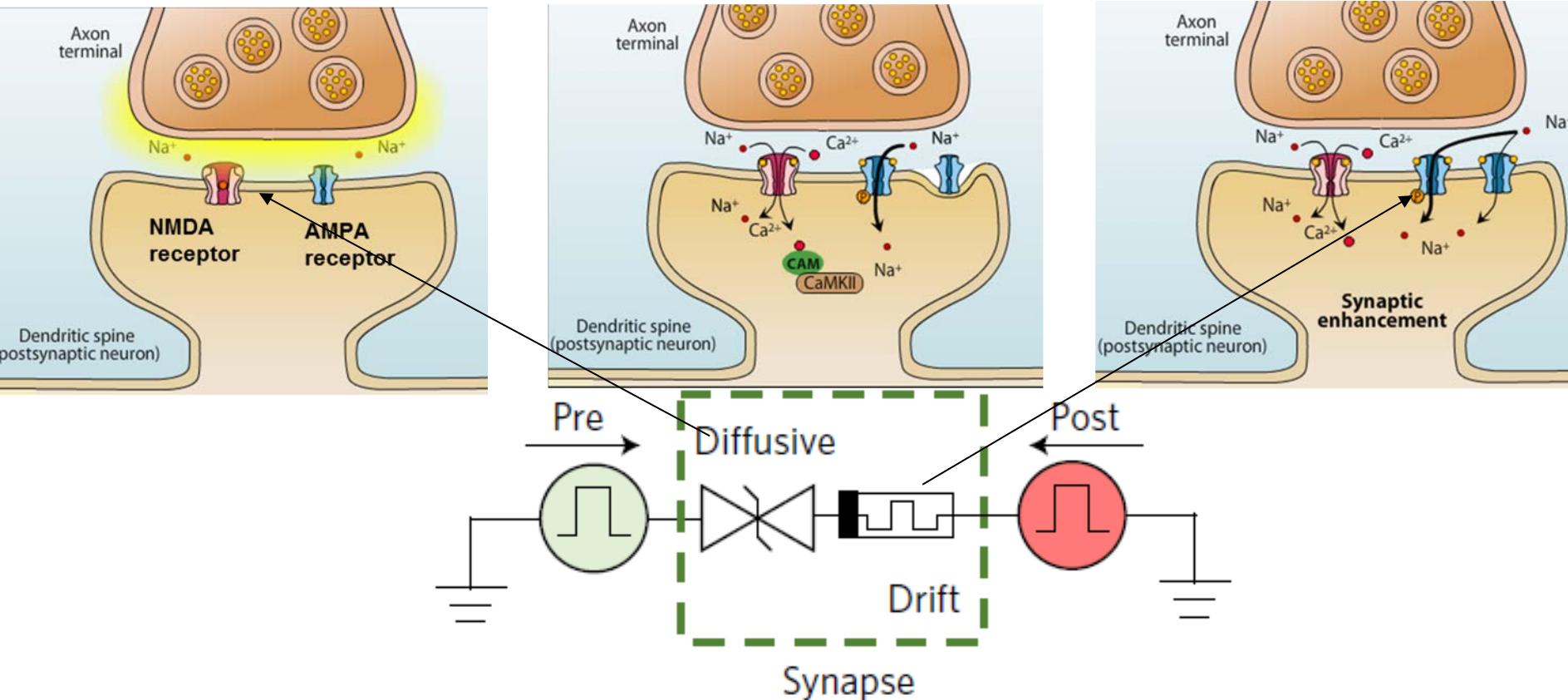


The Ca diffusion dynamics control the process!

<http://sites.sinclair.com/neuroscience5e/animations05.01.html>

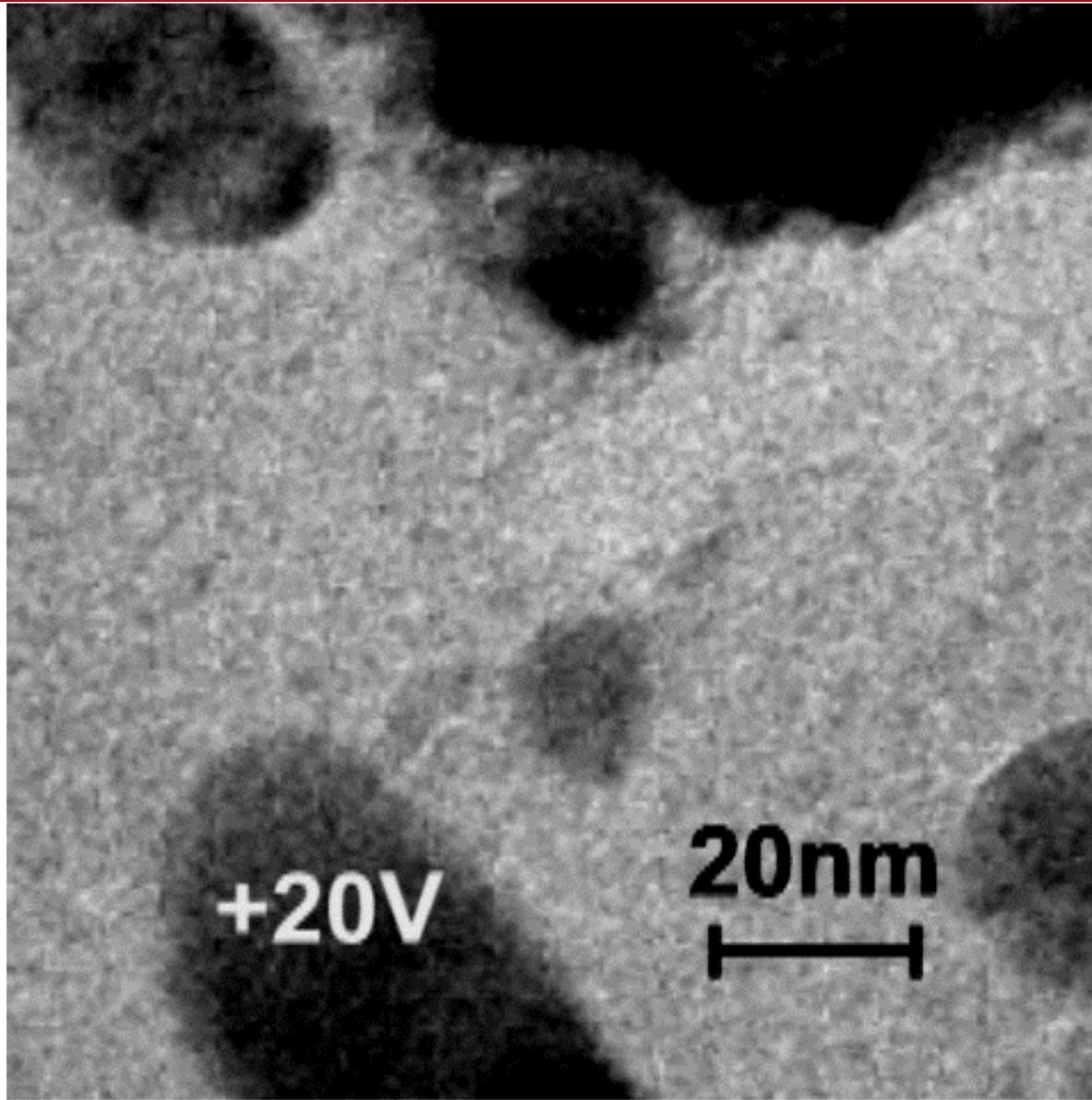
# Diffusion dynamics is critical for neuromorphic functions

**Very Large** Impulse from upper axon terminal → open NMDA receptor,  $\text{Ca}^{2+}$  diffuses through  
→ activate some bio-activities → increasing both the number and conductance of AMPA  
receptors → synapse enhanced – long term plasticity.



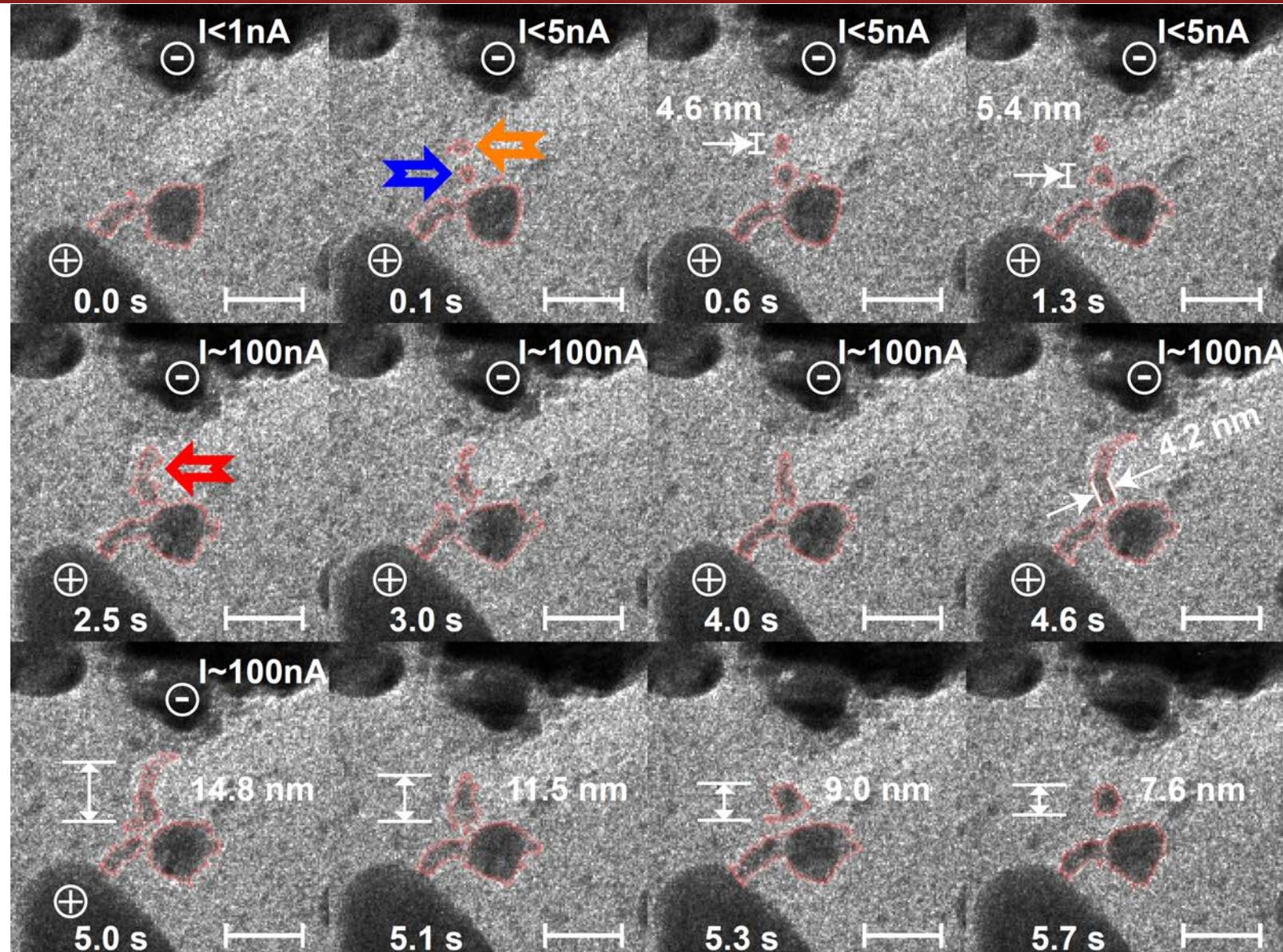
The  $\text{Ca}^{2+}$  dynamics controls the synaptic weight changes!

# Diffusion dynamics in Diffusive memristors

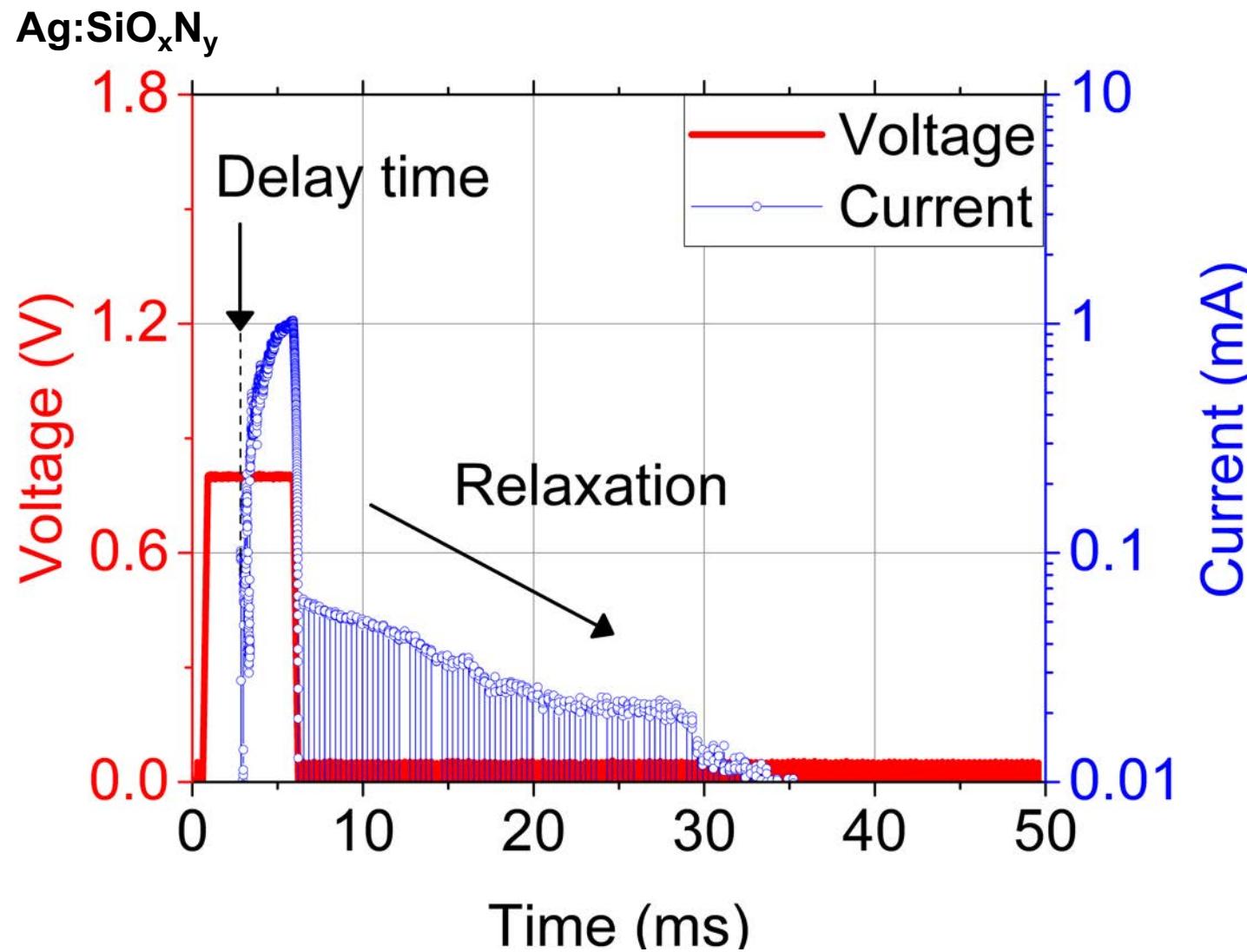


Z. Wang *et al.*, Nature Materials 16,  
101 (2017)

# Thermal diffusion and Interfacial energy minimization



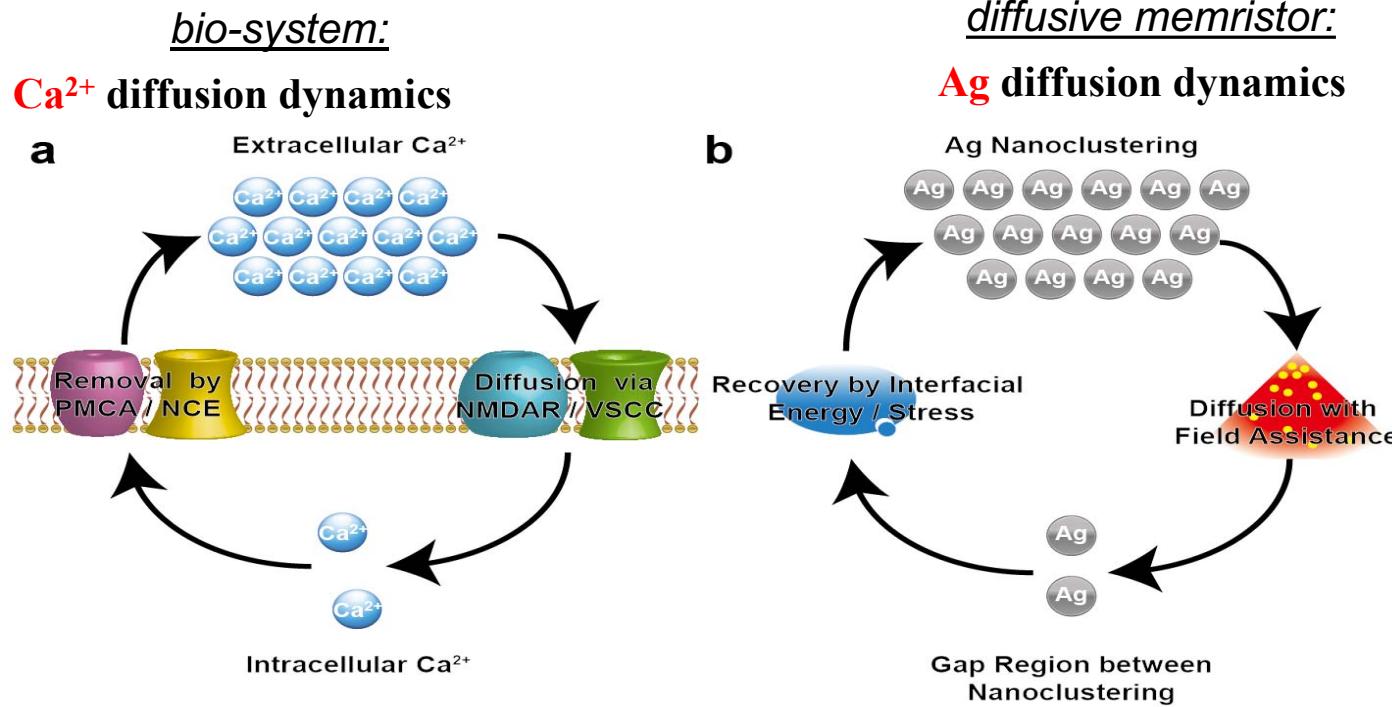
# Diffusive memristors: dynamics governed by thermodynamics



Z. Wang et al., Nature Materials 16, 101 (2017)

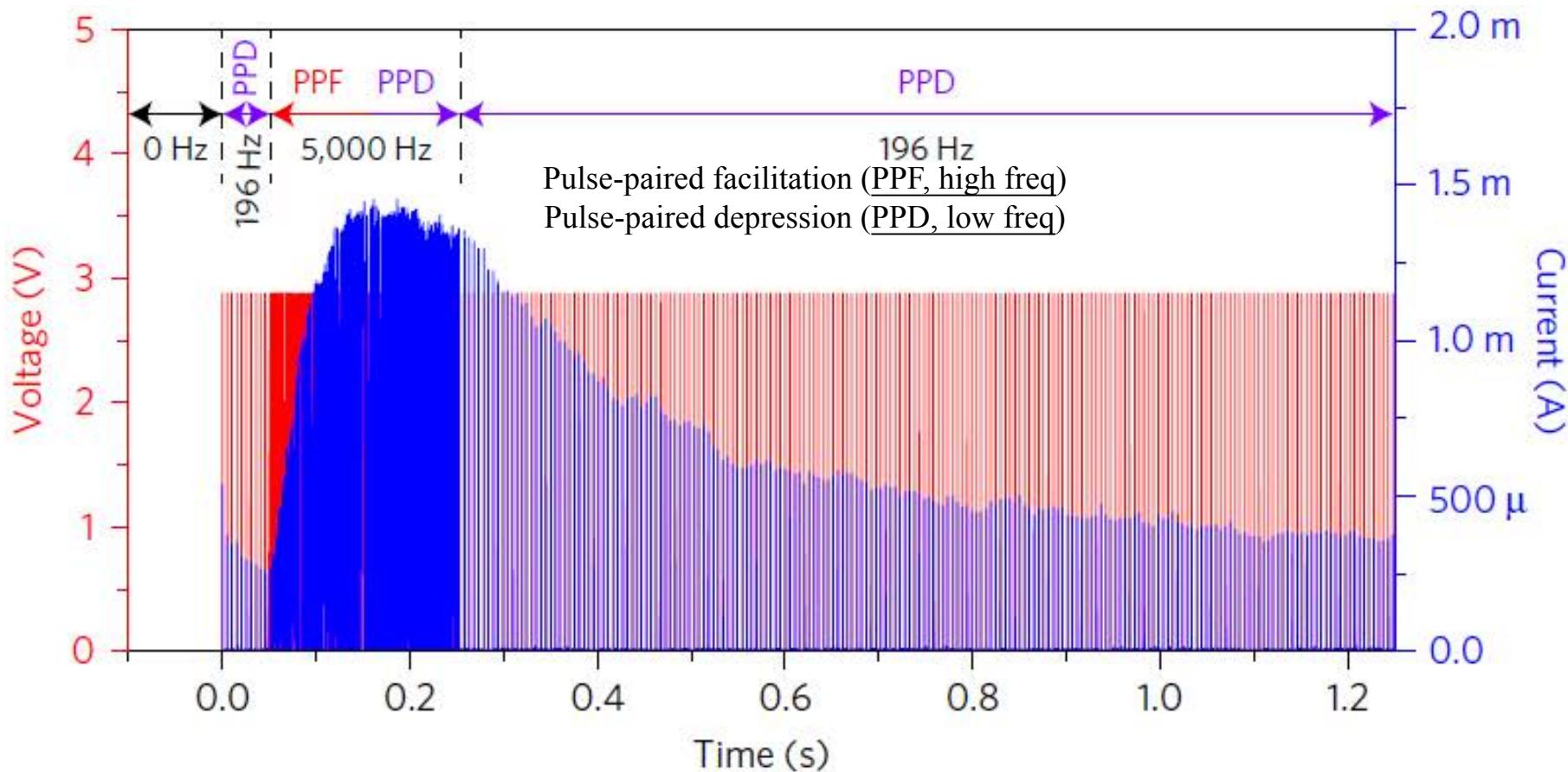
# Realization of critical Dynamics in memristors: (Ca/Ag diffusion analogy)

How to realize the critical dynamics:  
Physical similarity leads to mechanism and function similarities!!



# Artificial synapse:

## Realizing Short-term plasticity behavior faithfully



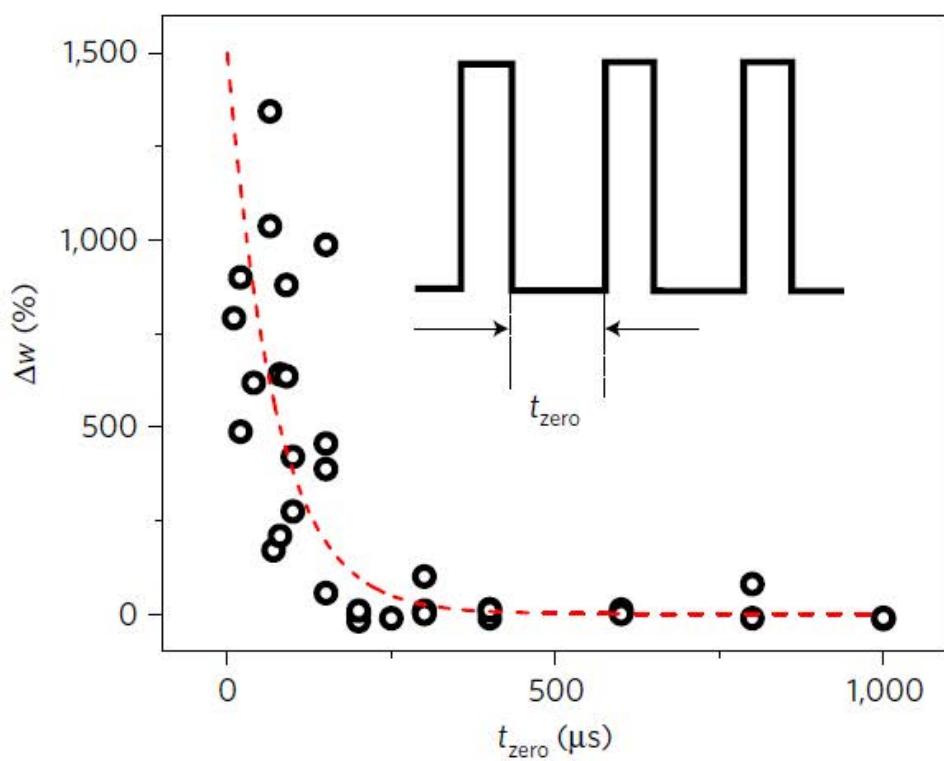
Naturally Reproduce synaptic behaviors long-observed in rat hippocampus!

(Dunwiddie, 1977)

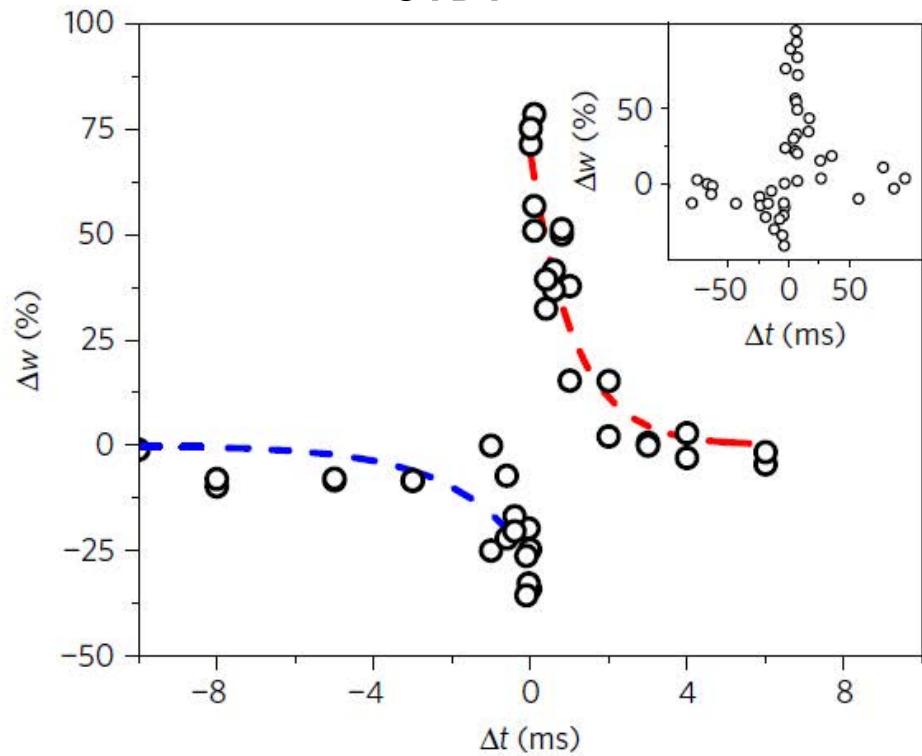
Z. Wang *et al.*, Nature Materials 16, 101 (2017)

# Artificial synapse: Realizing Long-term plasticity behavior faithfully

SRDP



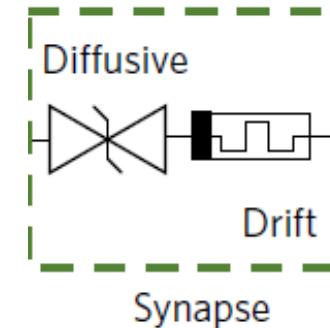
STDP



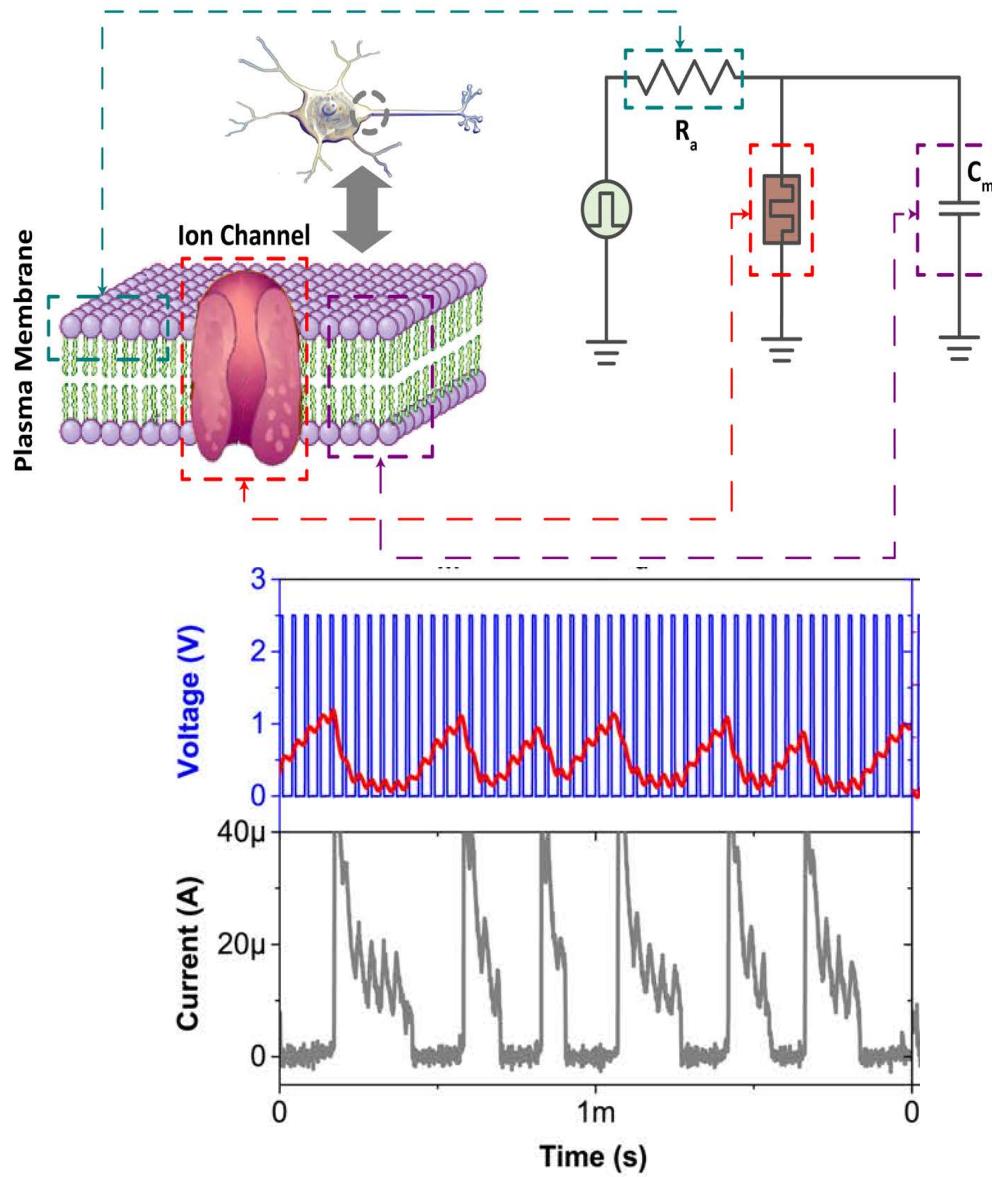
No pulse overlapping or stimulation engineering

Emulation with physical similarity (emulate many functions all together)  
instead of a pure phenomenological simulation (simulate one function a  
time)

Z. Wang et al., Nature Materials 16, 101 (2017)



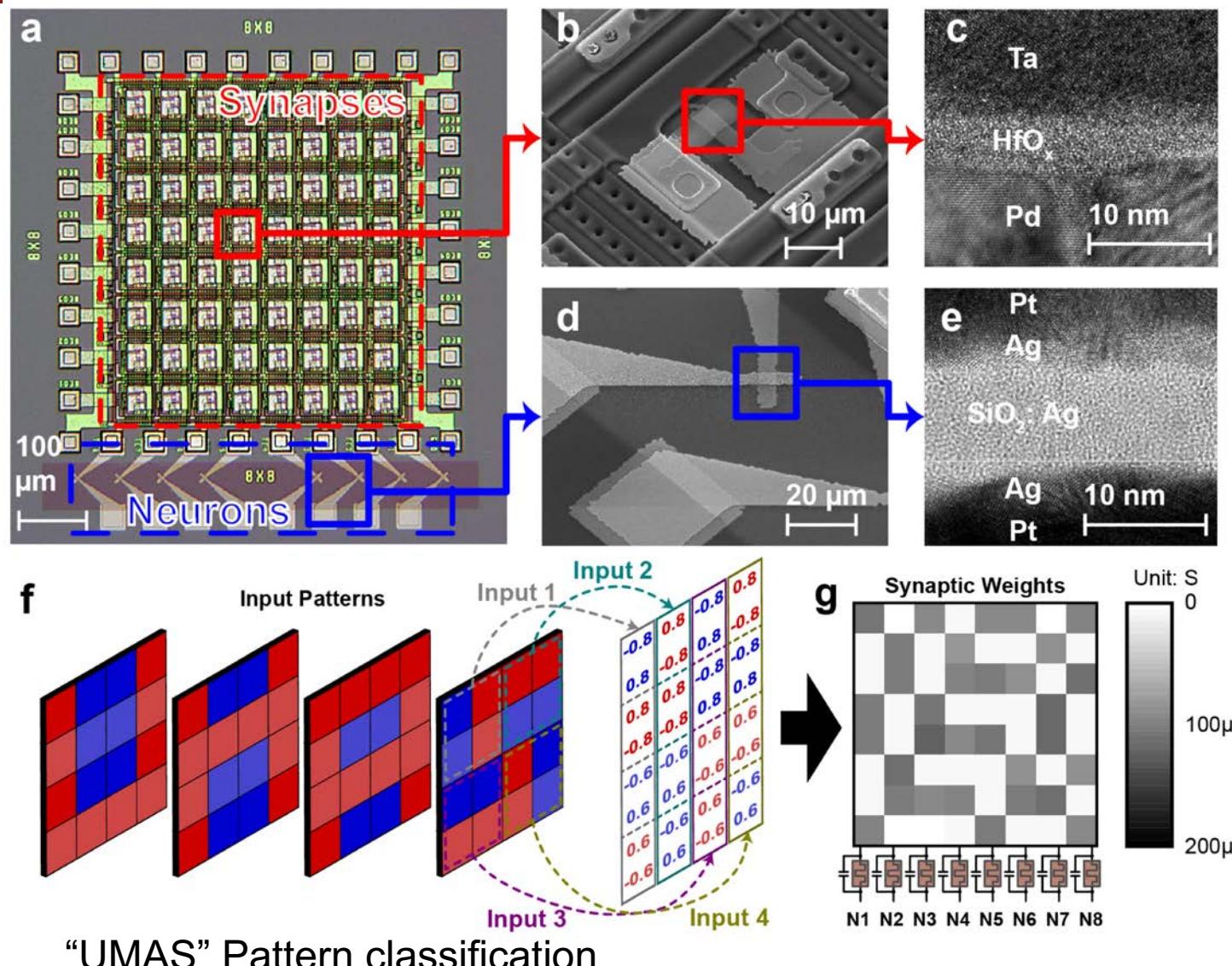
# Artificial neuron: leaky integration and fire with dynamics



Wang et al., *Nature Electronics* 1,137 (2018).

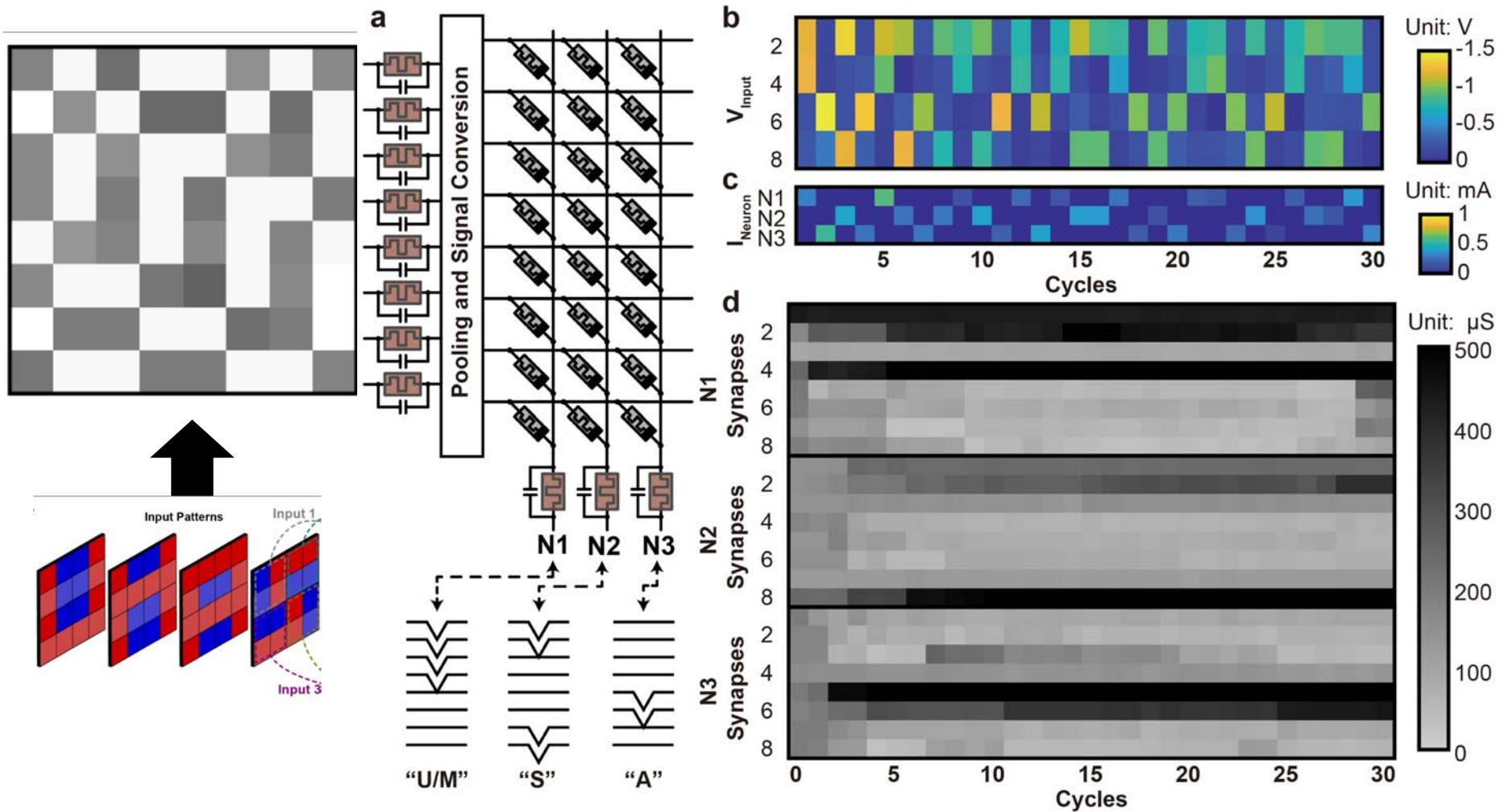
# **From device to neural networks (with thermodynamics)**

# 1<sup>st</sup> Integrated Fully Memristive Neural Network: Pattern Classification with Unsupervised Learning



Wang et al., *Nature Electronics* 1,137-145 (2018).

# 1<sup>st</sup> Integrated Fully Memristive Neural Network: Unsupervised Learning



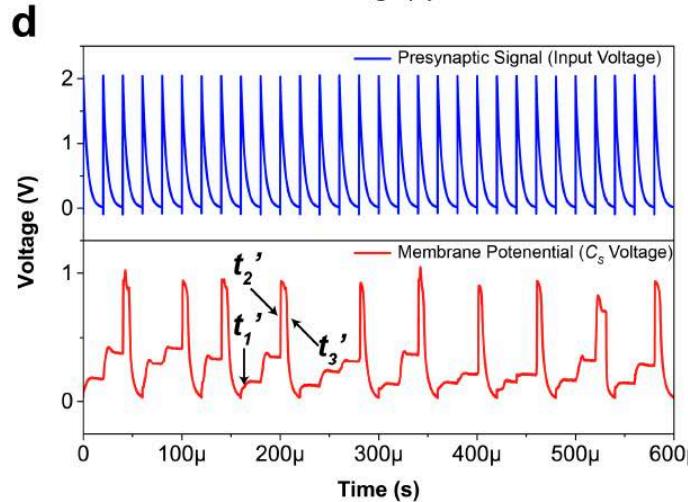
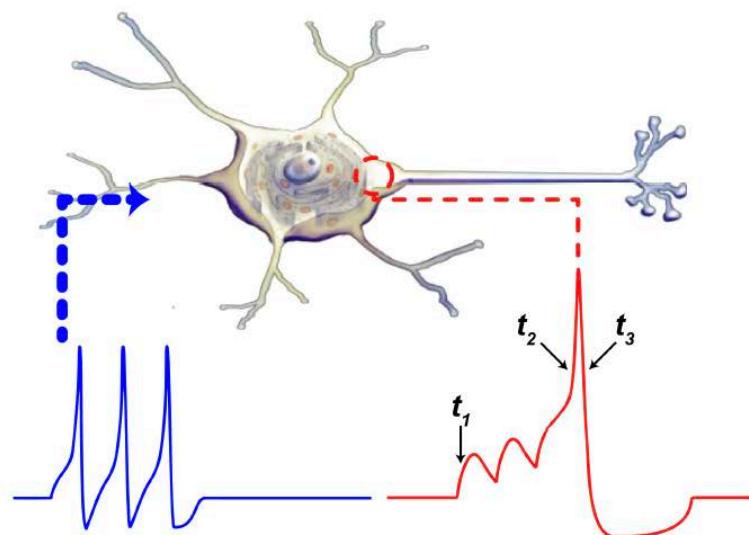
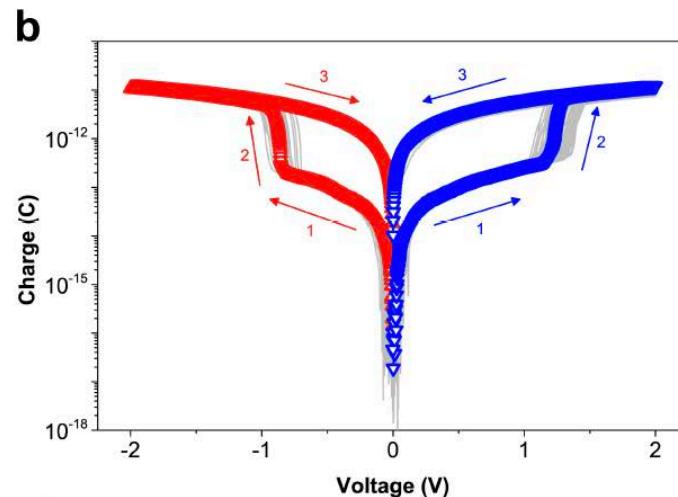
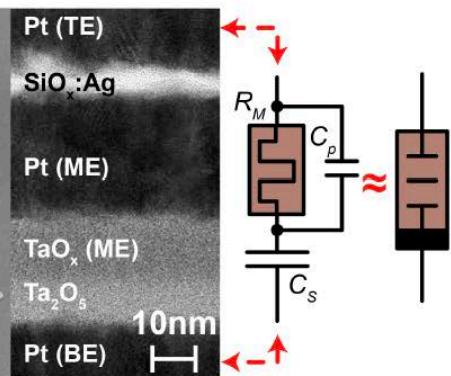
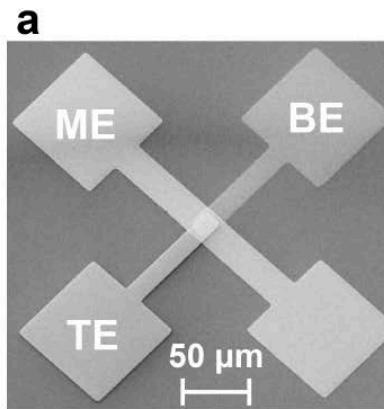
Example of Self-organization

Wang et al., Nature Electronics 1,137-145 (2018).

# Capacitive neural network?

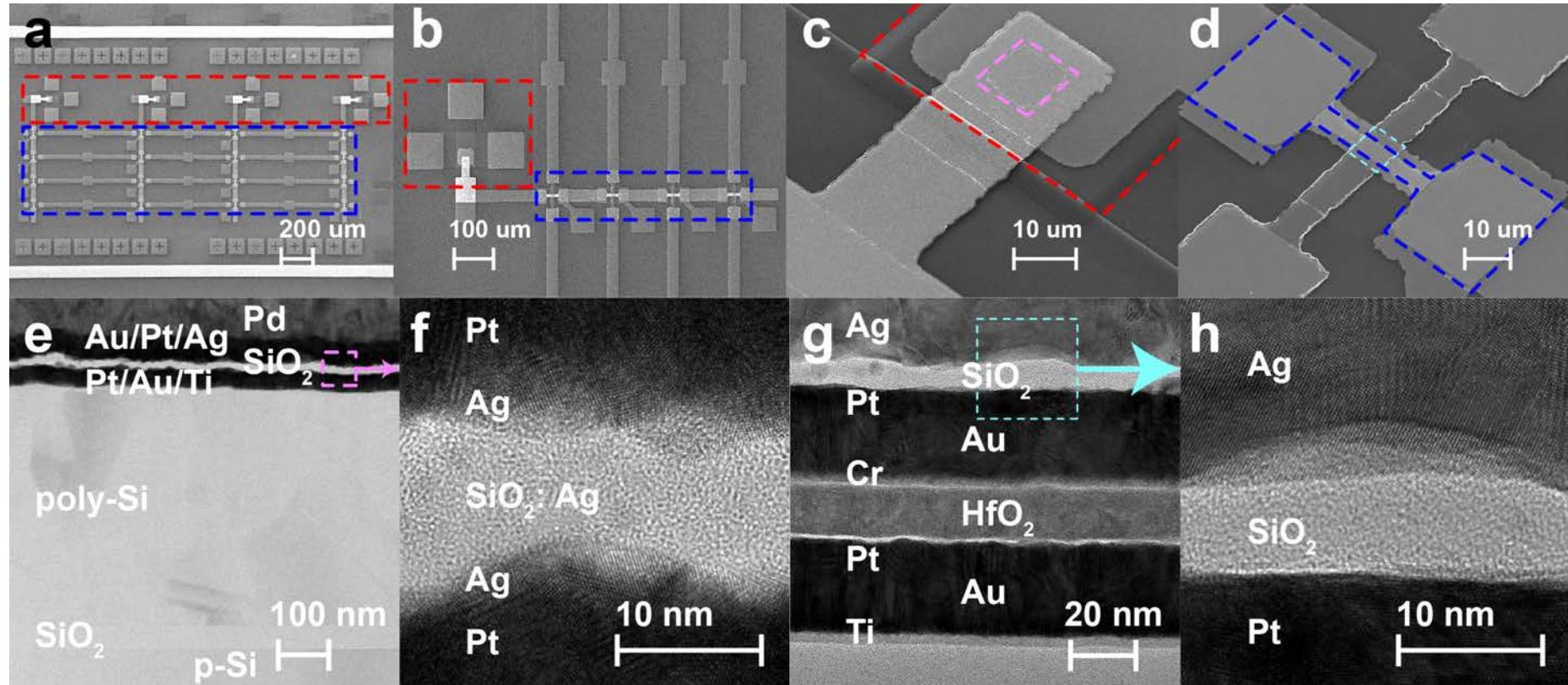
- No static current – less energy into heat;
- Recycle energy of electrical signals;
- Convenient for Spiking neural networks
- ...

# Pseudo – memcapacitor and neuro-transistor



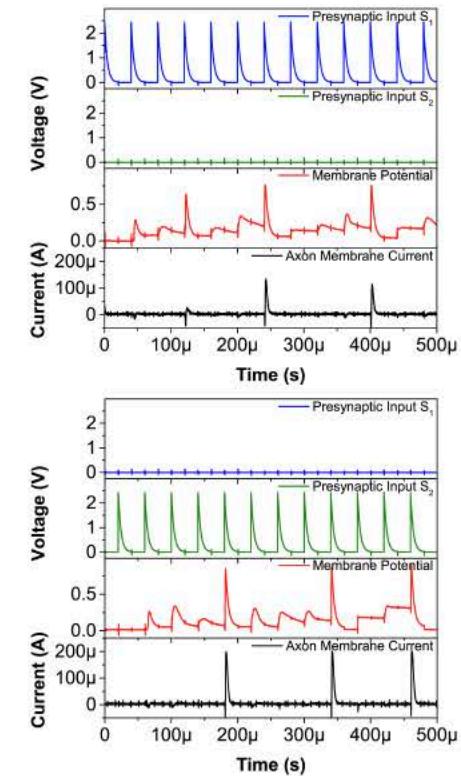
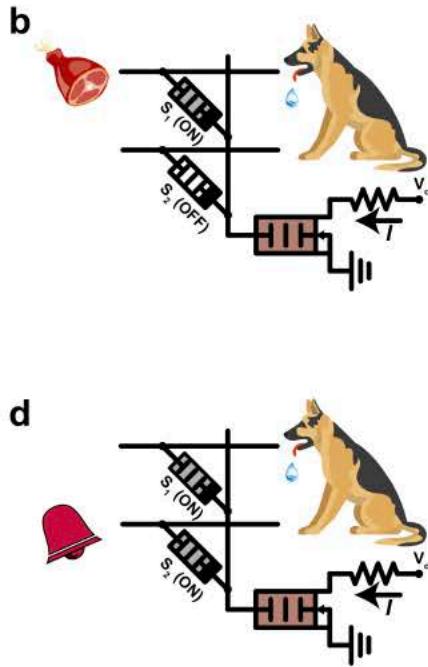
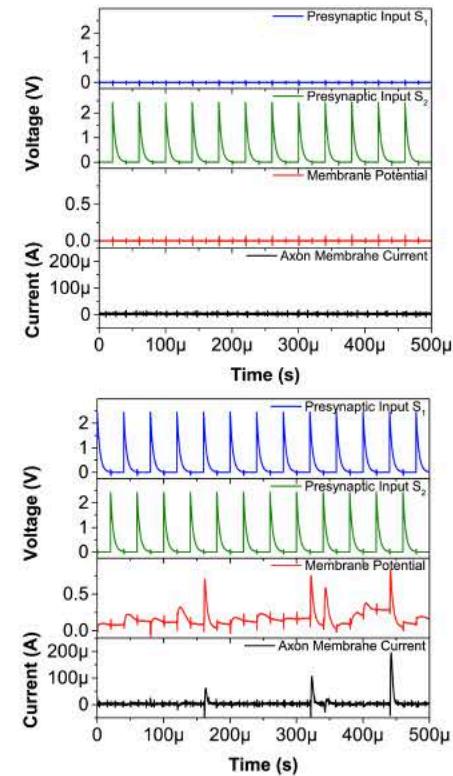
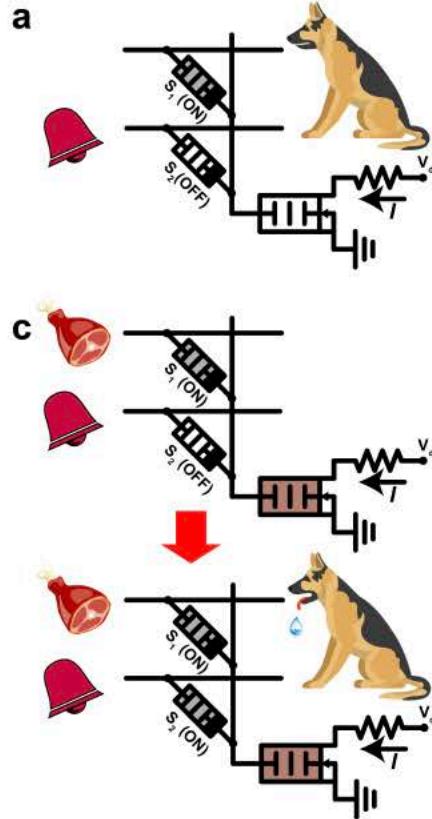
Wang et al., *Nature comm.* 9, 3208 (2018).

# a fully integrated capacitive neural network



Wang et al., *Nature comm.* 9, 3208 (2018).

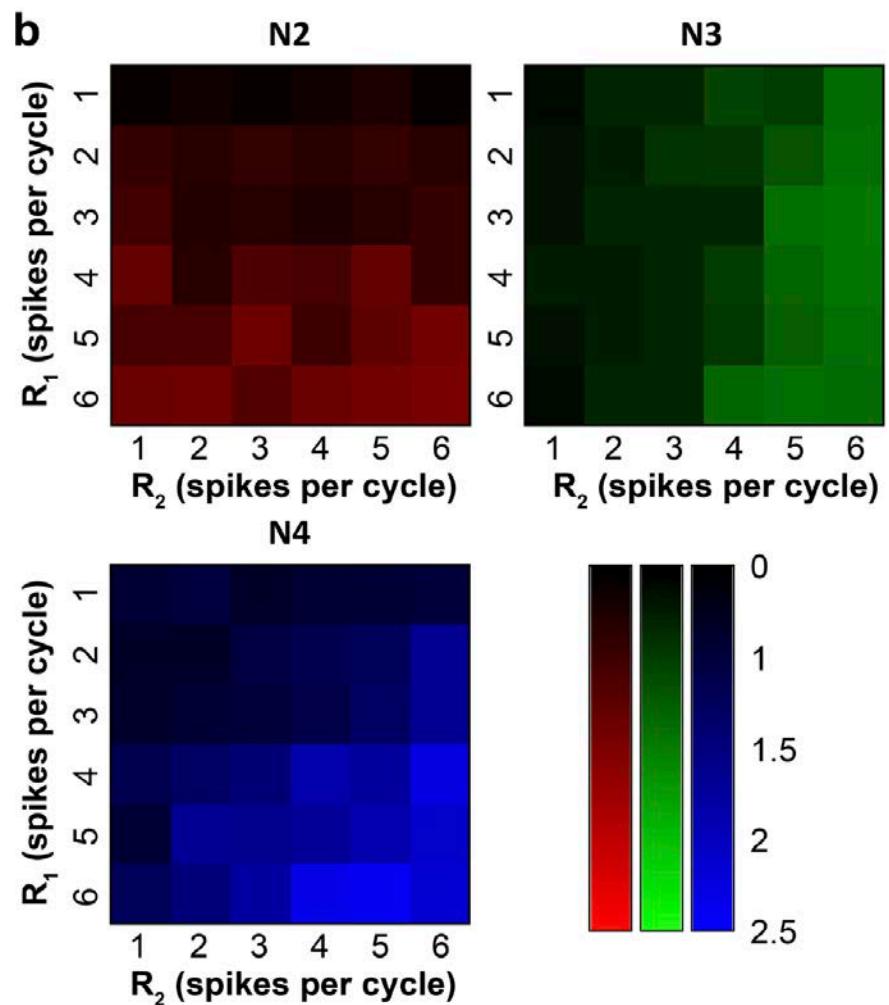
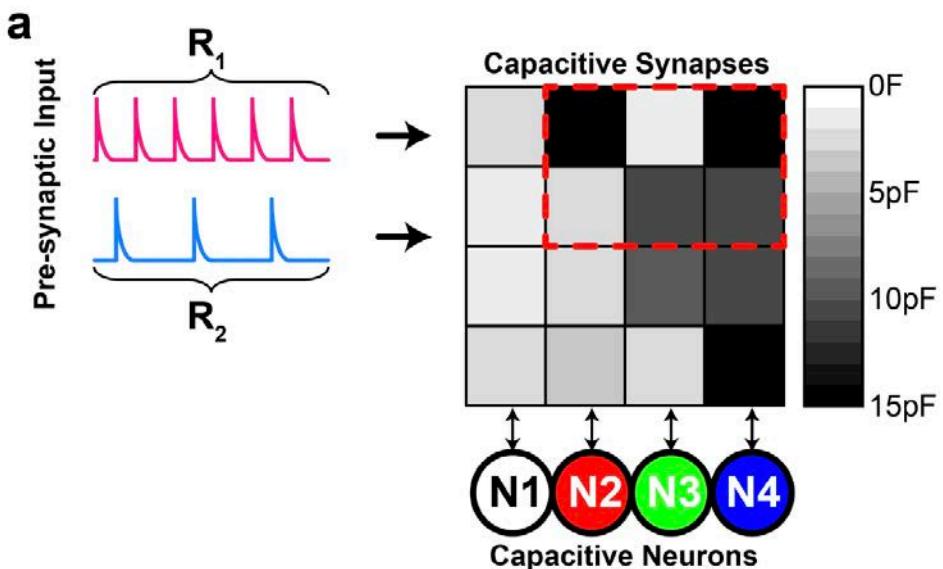
# Learning demonstration with capacitive neural network: Associative learning based on Hebbian-like mechanism



Wang et al., *Nature comm.* 9, 3208 (2018).

# Inference demonstration with capacitive neural network: Classification of spiking signals with different frequency

## Capacitive version of dot-product

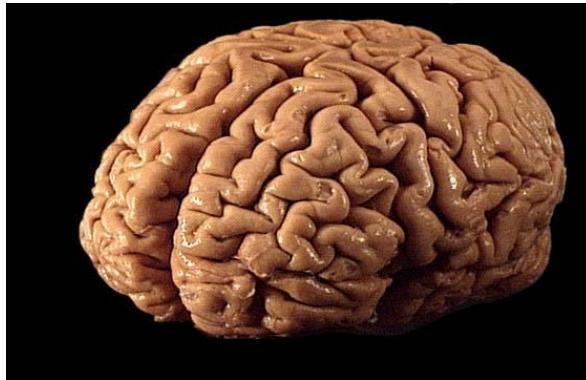


Wang et al., *Nature comm.* 9, 3208 (2018).

# Other potential physical systems

# Implement Neural network with CMOS devices

The last computing frontier



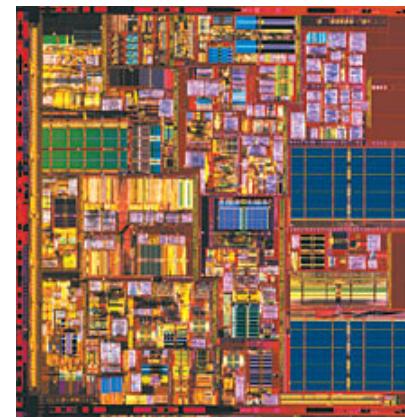
100 W

$10^{11}$  neurons

$10^{14-15}$  synapses

**1 Memristor = neuron**

**1 Memristor = synapse**



CMOS

100 W

$10^9$  transistors

10 transistors / synapse

$10^8$  synapses

$10^5$  neurons

Need  $\sim 10^7$  chips!!!

**Possible with nano memristors**

**Impossible with CMOS chips**

# Other physical systems: analog memories

	DRAM	FeRAM	MRAM	PRAM	Flash memory
Storage	Capacitor	Ferroelectric capacitor	TMR device	Phase-change device	Floating gate
Cell equivalent circuit	 Word line ————— Bit line	 Word line ————— Bit line	 Word line ————— Bit line	 Word line ————— Bit line	 Word line ————— Source Word line ————— Drain
“1” storage device	 +++++	 +++++	 Magnetization direction → ←	 Amorphous state	 Control gate
“0” storage device	 -----	 -----	 ← ←	 Crystalline state	 Floating gate
Advantages	<ul style="list-style-type: none"> <li>• High-speed write/read</li> <li>• Low cost</li> </ul>	<ul style="list-style-type: none"> <li>• Non-volatile</li> <li>• Low current consumption</li> <li>• Medium-speed write/read</li> </ul>	<ul style="list-style-type: none"> <li>• Non-volatile</li> <li>• Effectively infinite number of rewrites</li> <li>• High-speed write/read</li> </ul>	<ul style="list-style-type: none"> <li>• Non-volatile</li> <li>• Easy to manufacture</li> </ul>	<ul style="list-style-type: none"> <li>• Low cost</li> <li>• Non-volatile</li> </ul>
Disadvantages	<ul style="list-style-type: none"> <li>• High standby current</li> <li>• Volatile</li> </ul>	<ul style="list-style-type: none"> <li>• Scalability (not easy to port to smaller line widths)</li> <li>• Destructive read</li> </ul>	<ul style="list-style-type: none"> <li>• High write current</li> </ul>	<ul style="list-style-type: none"> <li>• High write current</li> <li>• Fewer rewrites than MRAMs, FeRAMs, etc</li> <li>• Rewrite slower than MRAMs, FeRAMs, etc</li> </ul>	<ul style="list-style-type: none"> <li>• Slow write</li> <li>• <math>10^5</math> or fewer rewrites</li> </ul>

# Take home messages

- **Bio-intelligent systems** may have a significant component of thermodynamic computing.
- Simple computing, such as inference after supervised learning, can be accelerated by neural networks of memristors **without much thermodynamics** involved. (**just a programmable network**)
- More advanced computing, such as pattern classification with unsupervised learning, can be achieved in neural networks of memristors functioning **based on thermodynamics**. (possible to generate **real intelligence**)
- Traditional Si devices were **not** created or optimized for thermodynamic computing; emerging devices, e.g. memristor, MRAM, FeRAM, PCM, FLASH are promising.
- Higher **energy efficiency** and **throughput** as well as **real intelligence** might be expected in those new computing paradigms.

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- Huolin L. Xin, Brookhaven National Laboratory
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