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Atomistic Modeling of Memristive Switching Mechanisms in Transition Metal Oxides

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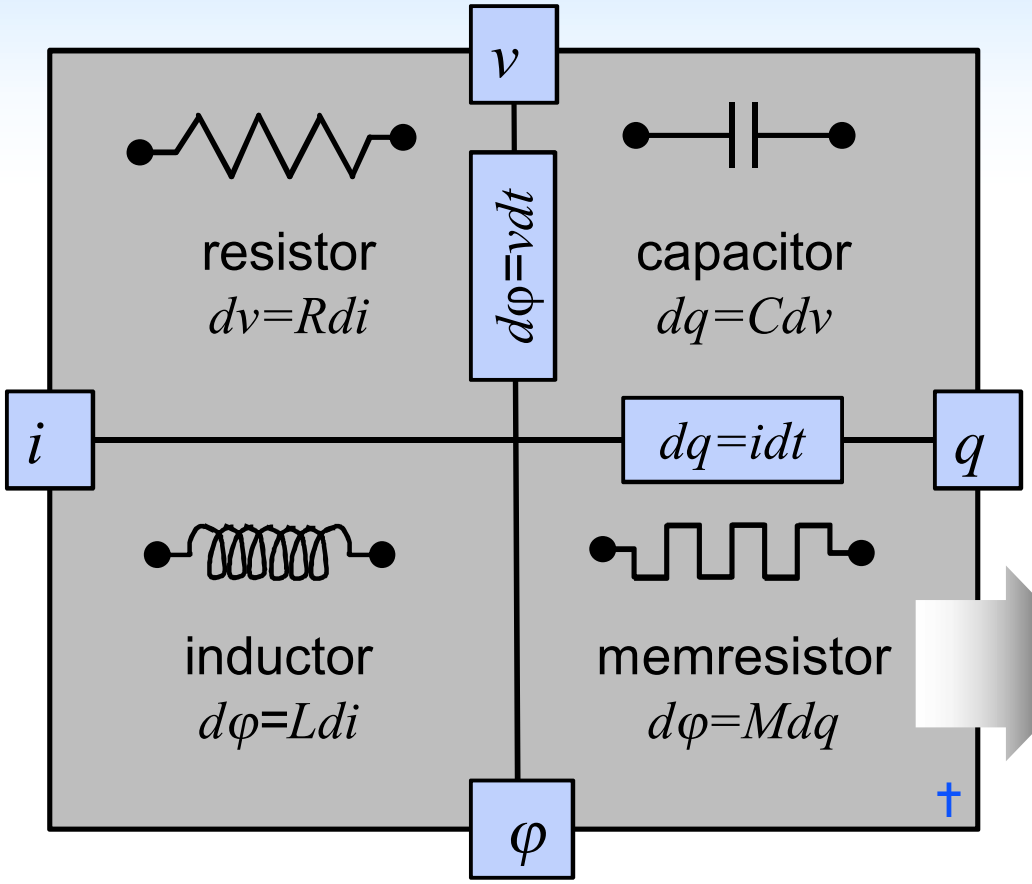
What is a Memristor?

- Leon Chua proposed[§] the 4th passive circuit element in 1971
- Device resistance changes as the integral of charge passed; hence, it "remembers" and retains the last resistance value (Ω) of energized ($i > 0$) circuit
- *i-v* behavior is hysteretic and reversible



- *M* is memristance
- What if *M*=*M*(*q*)?
- $M(q) \propto 1/d^2$

[†]Strukov, *Nature* **453**, 80 (2008).

[§]Chua, *IEEE Trans. Circuit Th.* **18**, 507 (1971).

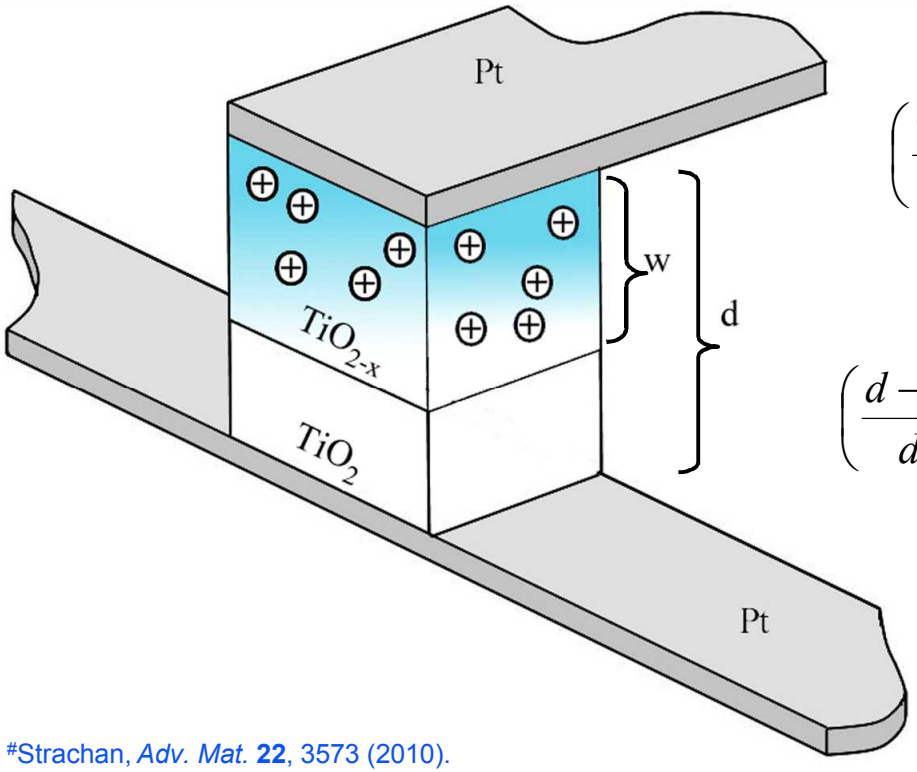
Memristor Applications

- **Non-volatile Memory (NVM)**: Memristor implementations known as resistive RAM (RRAM). NVM market currently dominated by Si-based Flash. Experimental RRAM devices meet/exceed Flash metrics:
  - *Density/scalability*[Δ§†] – crossbar architecture, feasible in 3-D. This is a path to **Pbit/cm^3** densities. (10s of Gbits possible in 25nm flash)
  - *Frequency*[§‡Δ] - < 10ns switch times (10μs in flash)
  - *Endurance*[§†] -10^{12} cycles (10^5 in flash)
  - *Retention*[§] – 10 years @ 85C observed (std. test)
  - *Low read/write voltages and energies*[‡] – 1 pJ switching
  - *Radiation hardness*[#]
- **Neuromorphic Design**[&%]: Non-linear, analog circuit designs mimicking biological systems (*i.e.* artificial brains, AI) enabled. Possible to implement synaptic behavior coupling axons and neurons in hardware. Synapses are essentially variable resistors.
- **Supercomputing**[%]: High-density memories are predicted enablers of massively-parallel, multi-core CPU architectures.

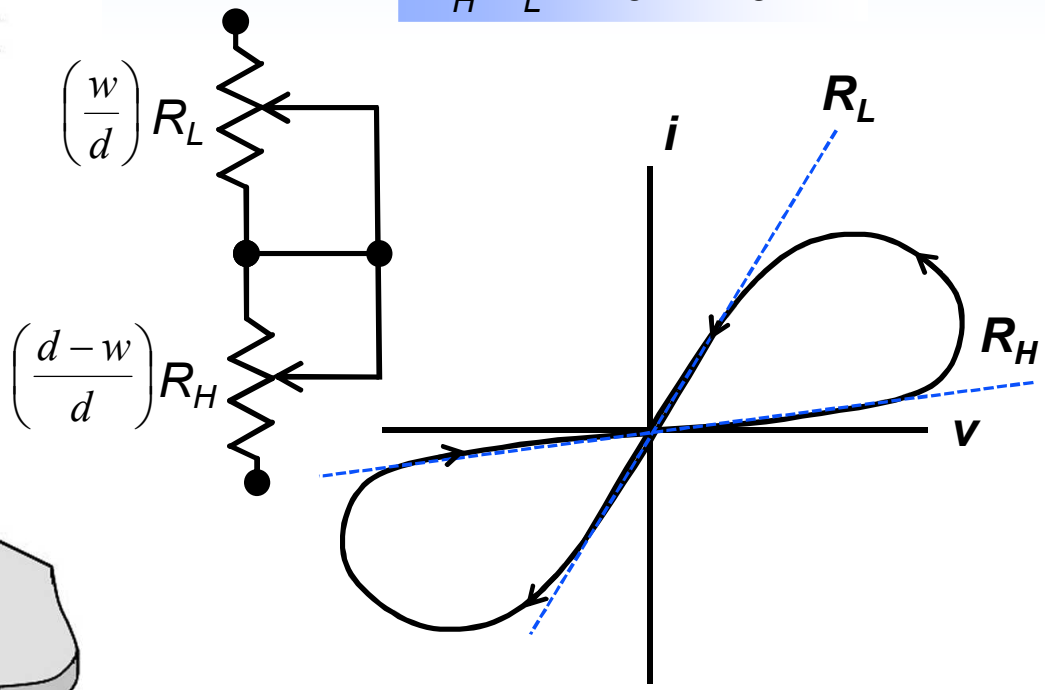
[%]Snider, *Computer* **44**, 21 (2011).
[Δ]Waser, *Adv. Mat.* **21**, 2632 (2009).
[†]Gerardin, *IEEE Trans. Nuc. Sci.* **57**, 3016 (2010)
[#]Tong, *IEEE Trans. Nuc. Sci.* **57**, 1640 (2010) .
[§]Lee, *Nature Mat.* **10**, 625 (2011).
[&]Williams, *IEEE Spectrum* **45**, 28 (2008).
[‡]Yang, *Appl. Phys. Lett.* **97**, 232102 (2010).

Memristor Physics

- In 2008, HP announced[†&] a memristor implemented in Pt/TiO_2/Pt. Behavior has since been generalized for many transition metal oxides and CMOS integration demonstrated.[‡]
- Mechanism believed to be driven by electrochemical redox reactions enabled by charged O vacancy (V_O^{2+}) migration; V_O^{2+} are immobile without electrical bias
- Phase change (stoichiometric and structural) dynamics at nanoscale remain elusive to experiment



$R_H/R_L \sim 10^2 - 10^3$ [#]

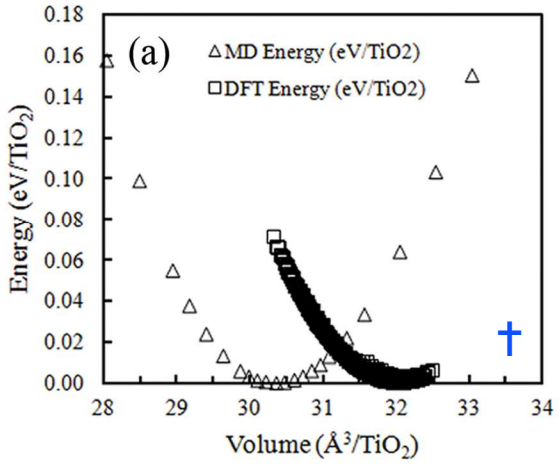


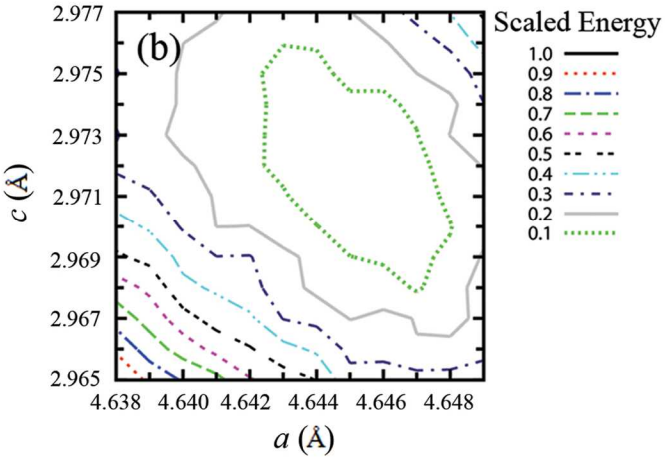
[#]Strachan, *Adv. Mat.* **22**, 3573 (2010).

[†]Strukov, *Nature* **453**, 80 (2008). [&]Williams, *IEEE Spectrum* **45**, 28 (2008). [‡]Xia, *Nano Lett.* 9, 3640 (2009).

Memristor Modeling: Challenges

- **Intrinsic Defects**: Are V_O the only critical contributors? Exact structure and charge states are essential. TiO_2 is relatively well-studied, but other MO_x (M = Ni, Nb, Ta, Cu, etc…)[Δ] systems are poorly understood.
- **Reliable Interatomic Potential**: Potentials must be developed capable of capturing essential defect dynamics. TiO_2 potentials are inadequate,[†] while published force fields do not exist[‡] for other systems like Ta_2O_5.
- **Material System**: TiO_2 has best knowledgebase, but phase diagram is complex. There are various polymorphs (rutile, anatase) plus thermodynamically-stable reduced Magnéli phases (Ti_nO_{2n-1}).[§] Ta-O phase diagram is simple; however, crystal structure is under debate, which will inhibit defect investigation.[#‡] Amorphous and nanocrystalline phases are likely relevant.
- **Computational Feasibility**: Large system size (>10^6 atoms) and timescales (~10ns) will be essential to capture switching dynamics.





[Δ]Waser, *Adv. Mat.* **21**, 2632 (2009).

[†]Matsui & Akaogi, *Molec. Sim.* **6**, 239 (1991).

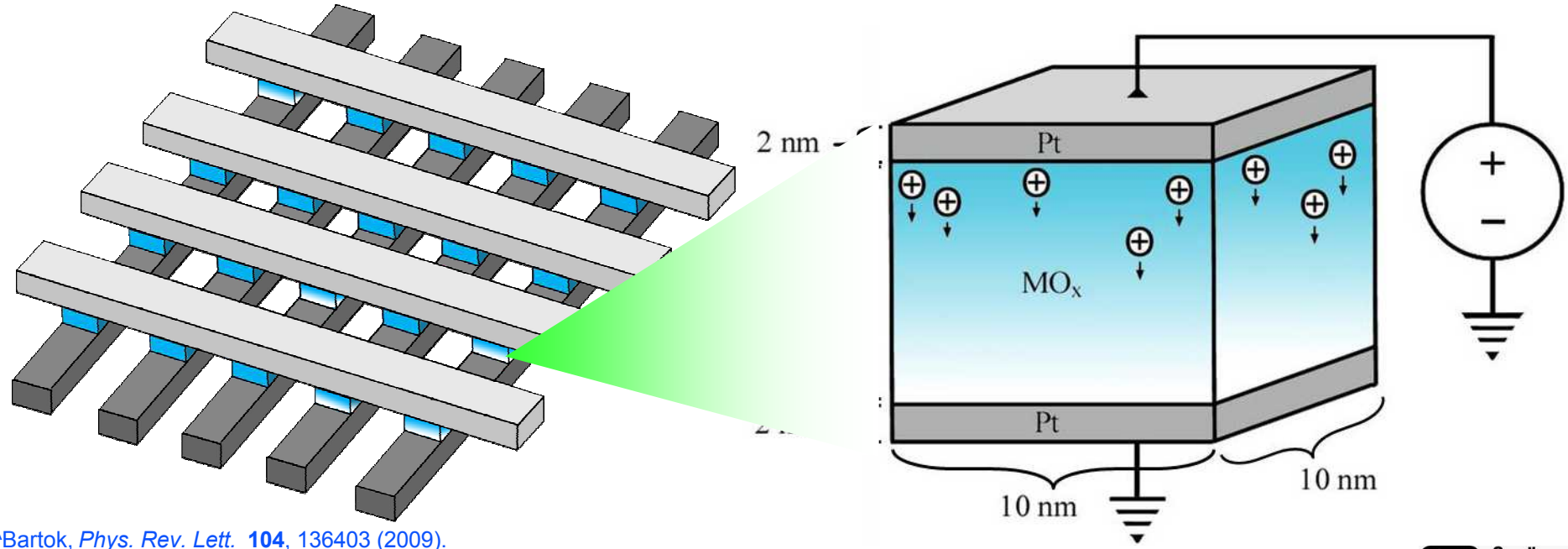
[‡]Wu, *Phys. Rev. B* **83**, 144105 (2011).

[§]Liborio, *Phys. Rev B* **77**, 104104 (2008).

[#]Yang, *Appl. Phys. Lett.* **97**, 232102 (2010).

Memristor Modeling: Strategy

- Determine/confirm structure and preferred oxidation state of dominant intrinsic defects in relevant phases with density-functional theory (DFT)
- Assess phase transition simulation feasibility in MO_x systems (TiO_x ,TaO_x , etc…)
- Develop & evaluate fidelity of potentials against DFT/experimental results. Interatomic potential classes include ReaxFF and Gaussian approx. potential (GAP).[Δ]
- Characterize defect behavior in LAMMPS under suspected driving conditions: electrical bias, temperature, and/or pressure/strain
- Atomistic LAMMPS simulation of relevant phase transition(s) (10^3 to 10^4 atoms)
- Atomistic LAMMPS simulation of memristor switching mechanism (10^5 to 10^6 atoms for ~ 10ns)



[Δ]Bartok, *Phys. Rev. Lett.* **104**, 136403 (2009).

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