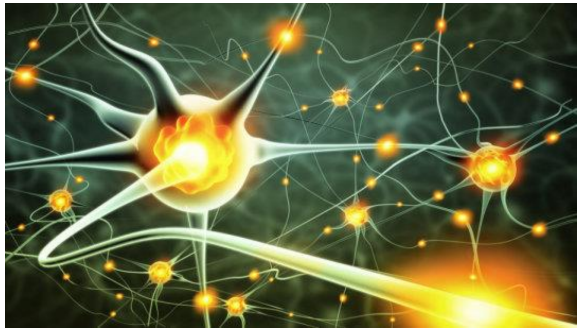
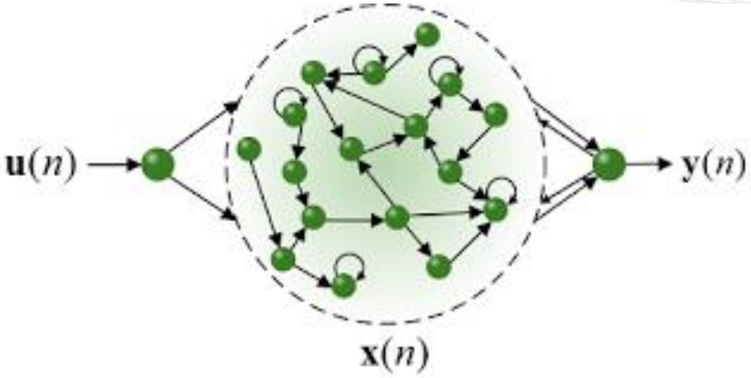
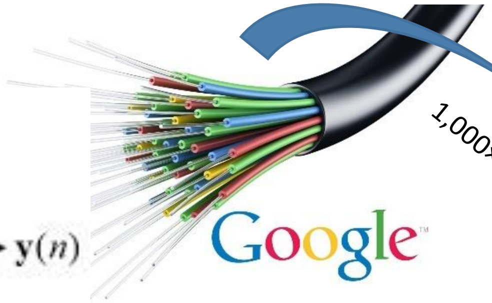
Optoelectronics with Oxides and Oxide Heterostructures



Alex Demkov

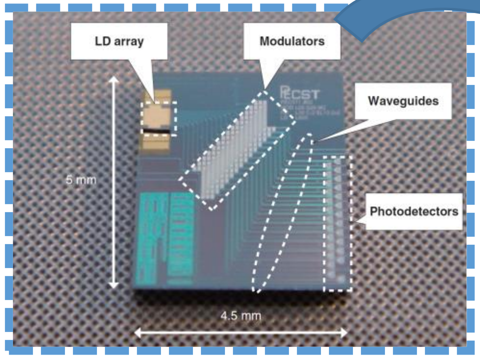
The University of Texas





1,000x Smaller

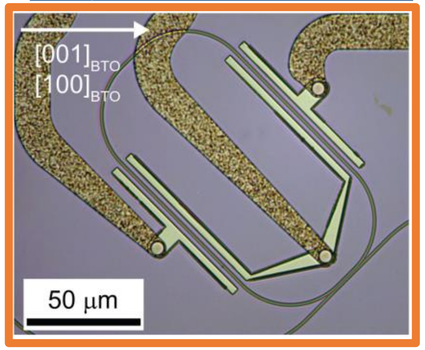
Si Photonics



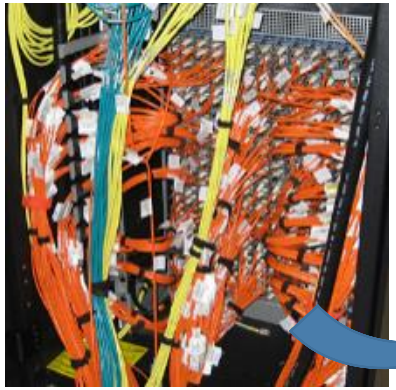
Si Photonics (10^{-3} m)

100x Smaller

Hybrid oxide/Si Photonics



Nanophotonics (10^{-5} m)

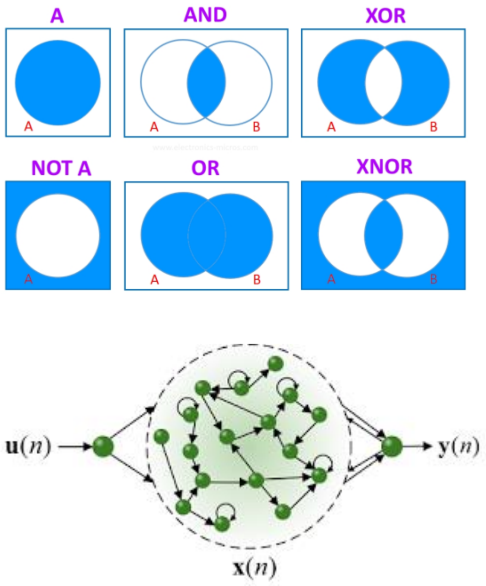


IBM Roadrunner (1 m)

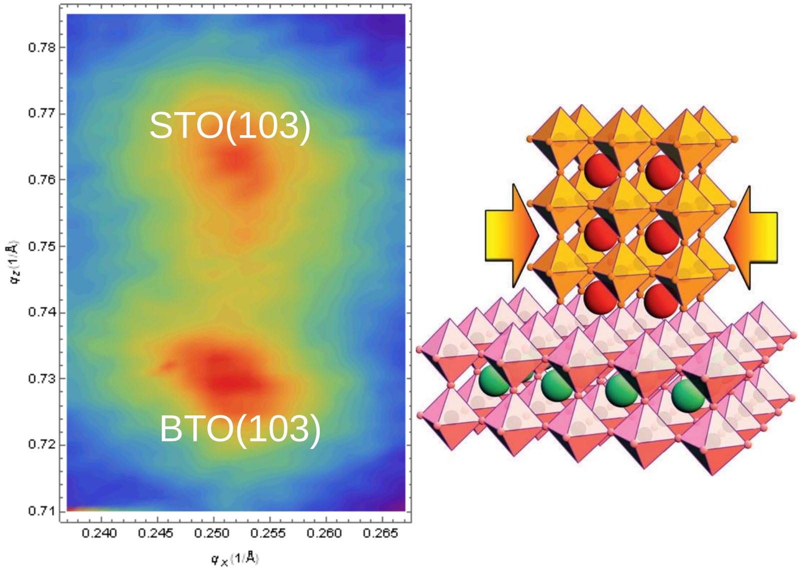
1,000x Smaller

Outline

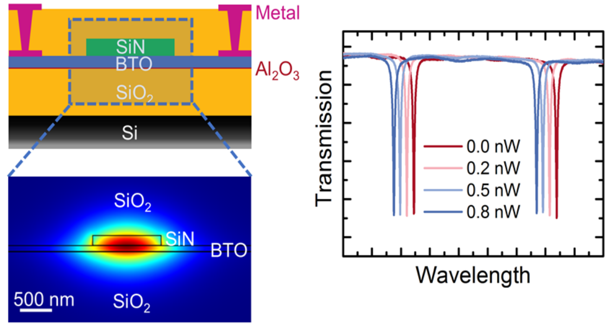
1. Introduction



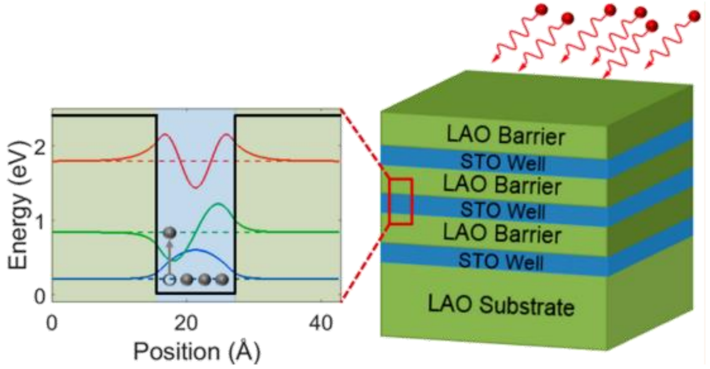
2. Oxides



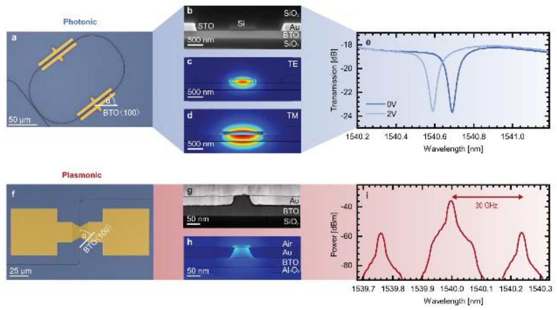
3. BTO Electro-Optic Devices



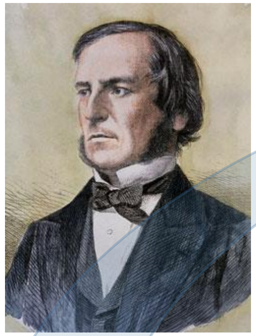
4. Oxide Heterostructures



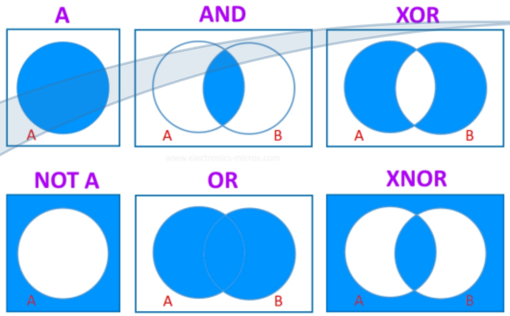
5. Conclusions



Traditional Computing

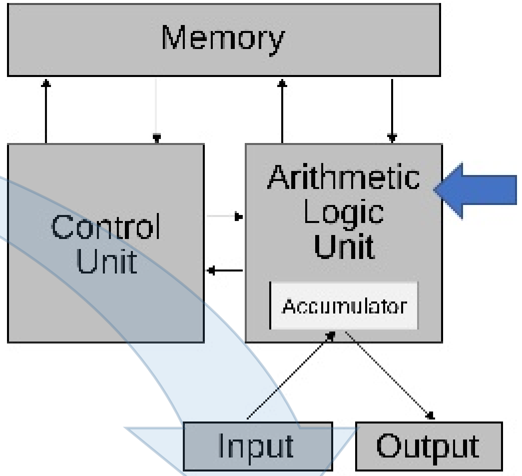


George Bool
1815 –1864

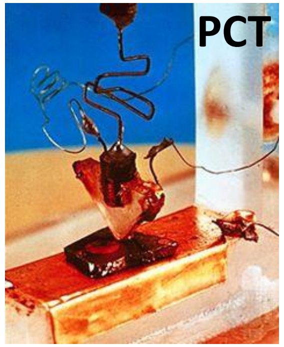


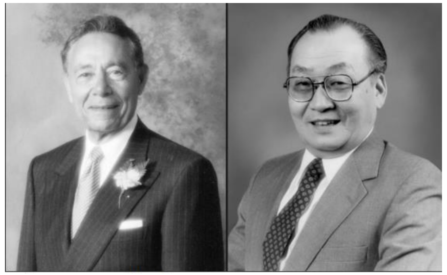
Boolean Algebra
1847

John von Neumann
1903 -1957



Von Neumann Architecture





M. Atalla & D. Kahng
1959

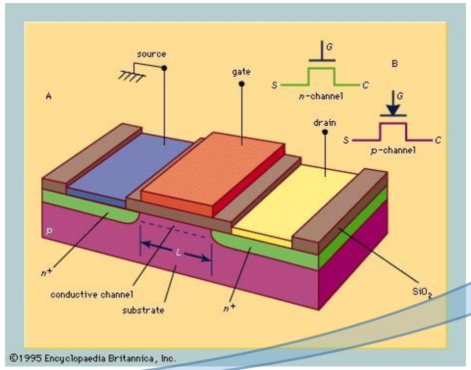
MOSFET

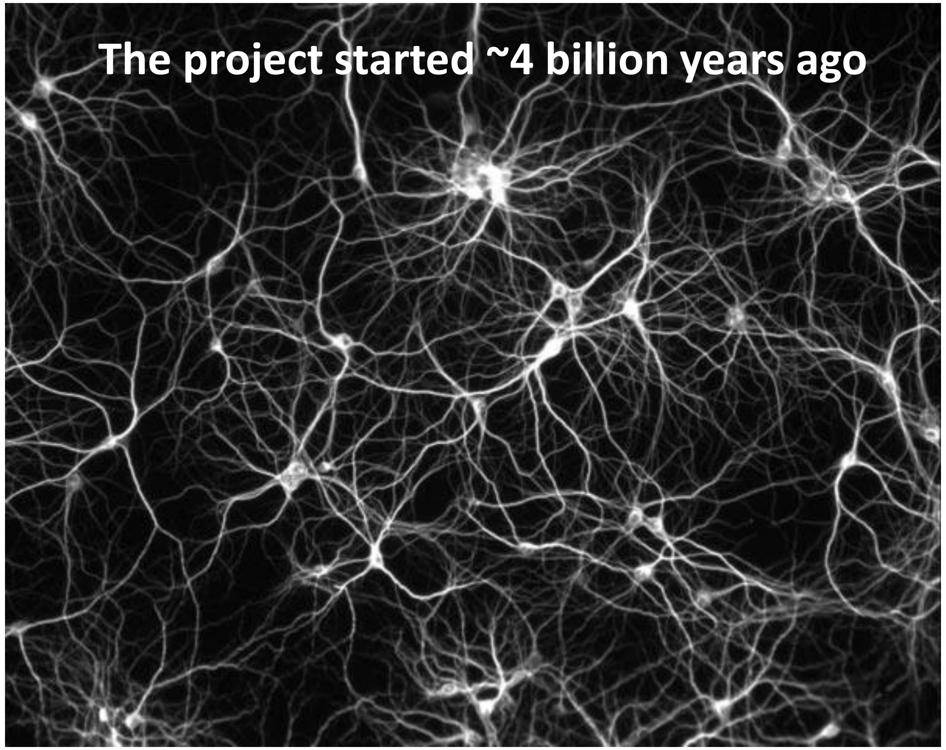
J. Kilby & R. Noyce
1970s

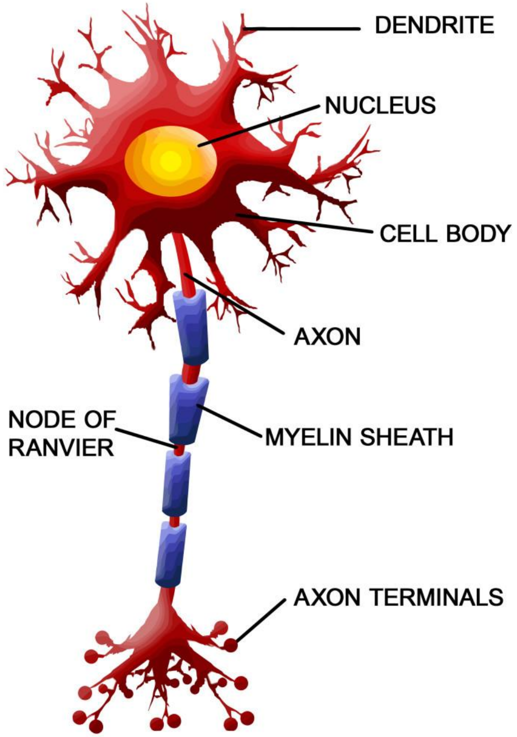
J. E. Lilienfeld
1925

FET

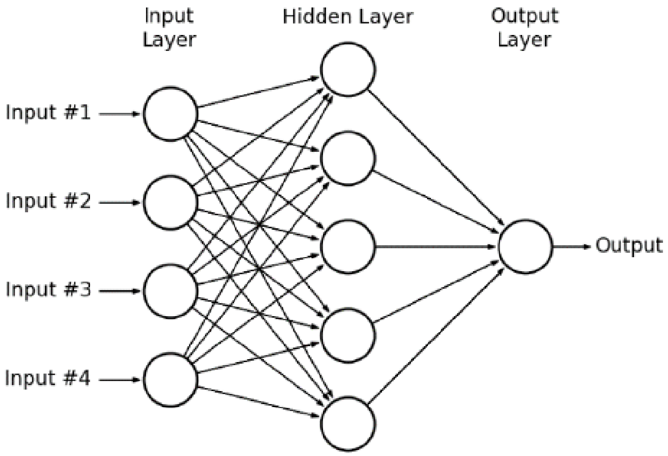
J. Bardeen, W. Brattain and W. Shockley
1947

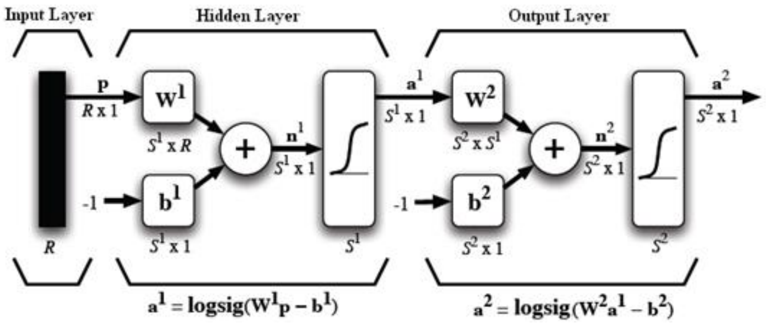




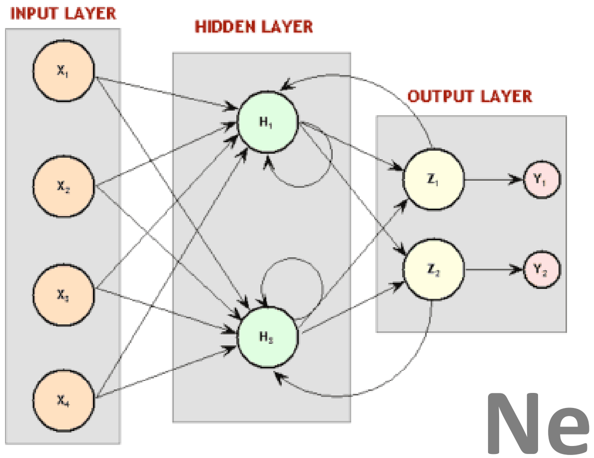


Feedforward network

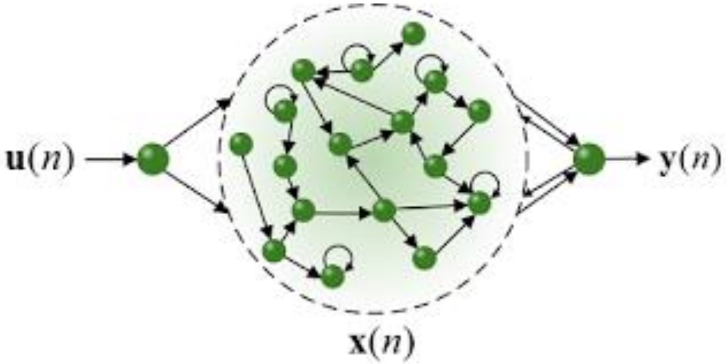




Recurrent network



Echo state network

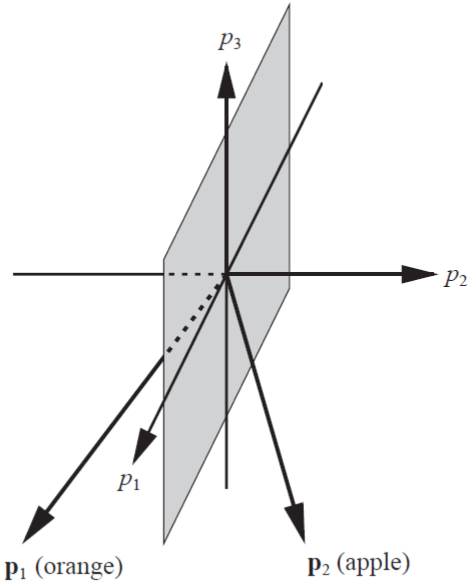


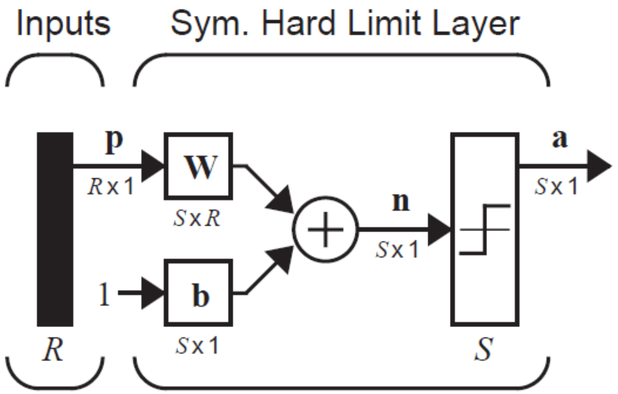
Neuromorphic Computing

A single-neuron perceptron

$$\mathbf{p} = \begin{bmatrix} shape \\ texture \\ weight \end{bmatrix}$$

$$\mathbf{p}_2 = \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} \qquad \mathbf{p}_1 = \begin{bmatrix} 1 \\ -1 \\ -1 \end{bmatrix}$$





$$\mathbf{a} = \mathbf{hardlims}(\mathbf{Wp} + \mathbf{b})$$

$$a = hardlims\left(\begin{bmatrix} w_{1,1} & w_{1,2} & w_{1,3} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix} + b\right)$$

$$a = hardlims\left(\begin{bmatrix} 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \\ -1 \end{bmatrix} + 0\right) = -1(orange)$$

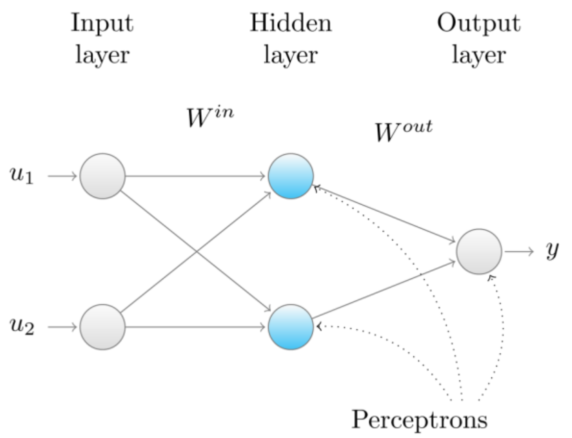
$$\mathbf{W} = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix}, \; b = 0 .$$

$$a = hardlims\left(\begin{bmatrix} 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} + 0\right) = 1(apple)$$

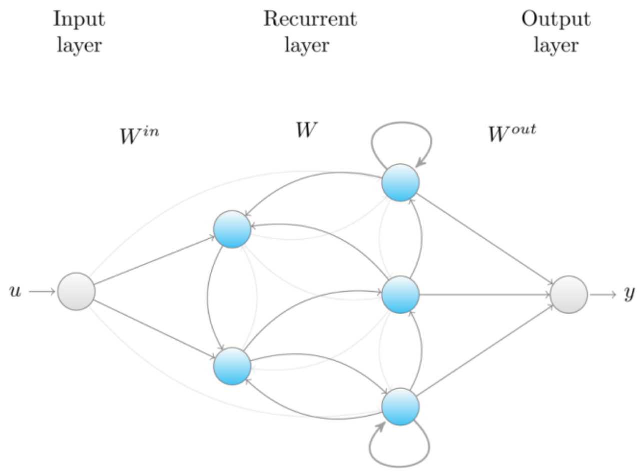
$$a = hardlims\left(\begin{bmatrix} 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix} + 0\right) = -1(orange)$$

ANN Taxonomy (a physicist's point of view)

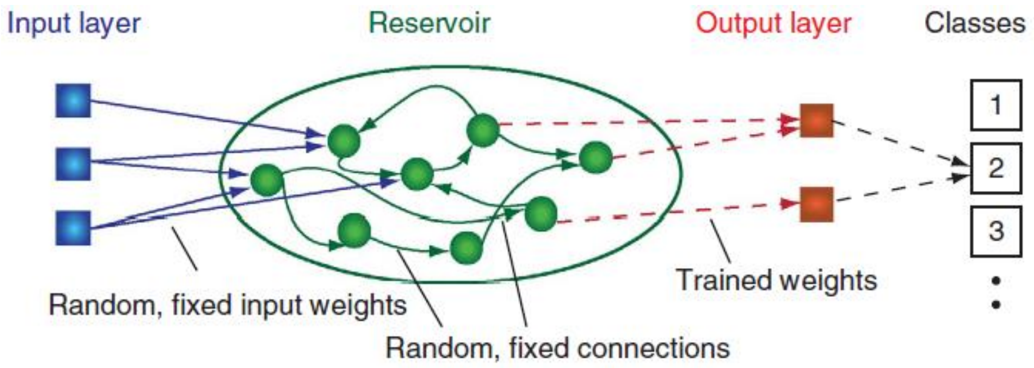
Feedforward neural network (FNN)



Recurrent neural network (RNN)



Reservoir Computer (RC)



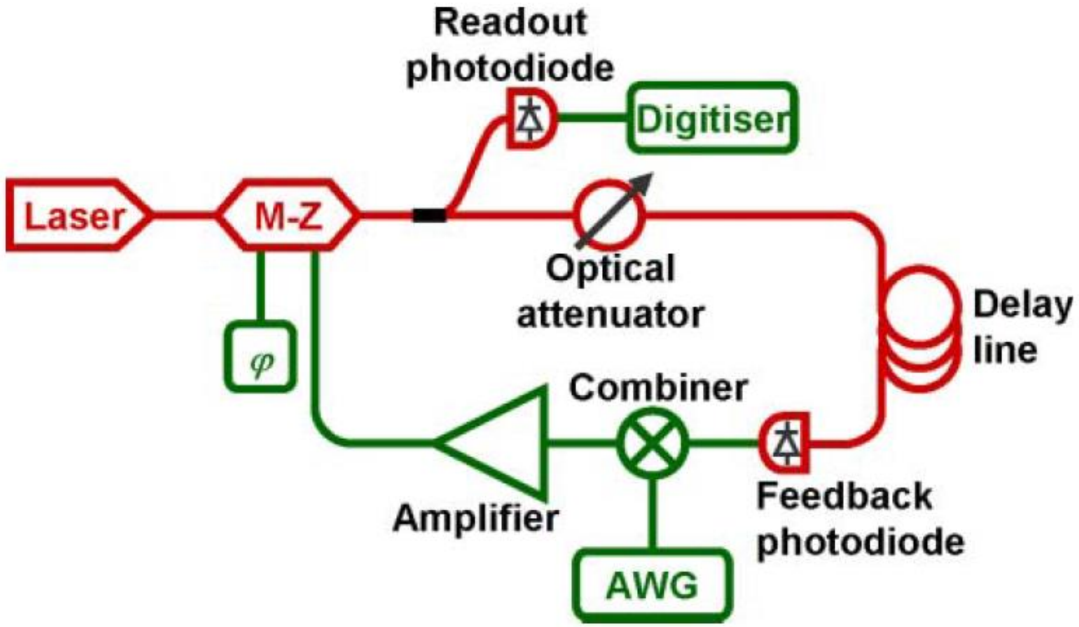
$$\mathbf{x}(n+1) = f\left[W^{in}\mathbf{u}(n+1) + W\mathbf{x}(n)\right], \quad n = 1, 2, \ldots, T,$$

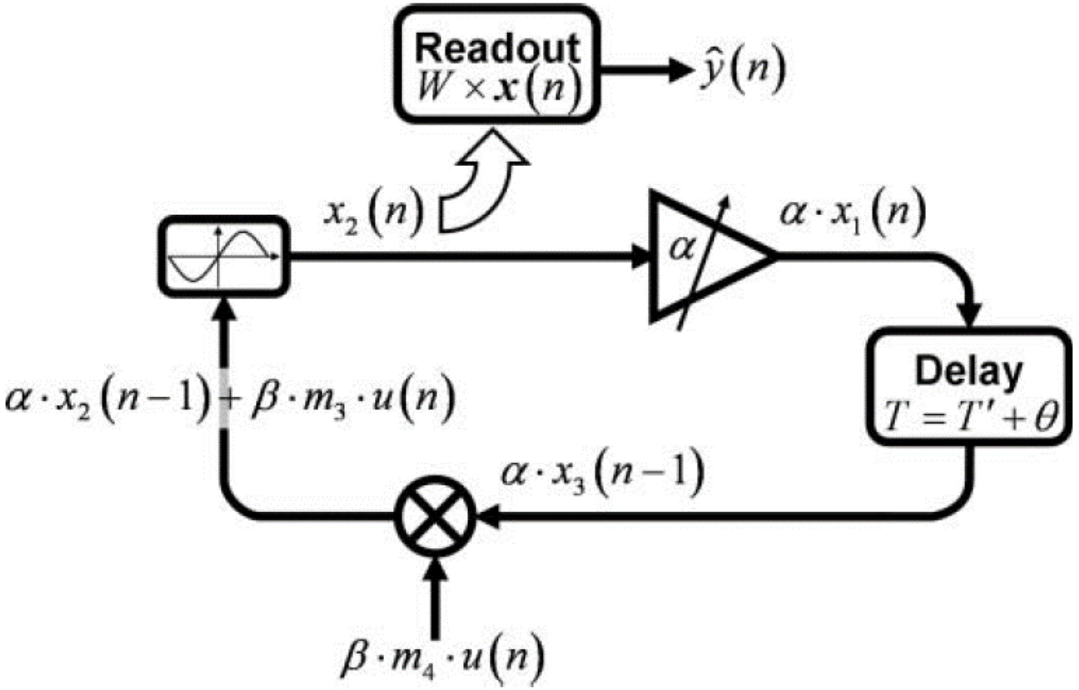
SCIENTIFIC REPORTS

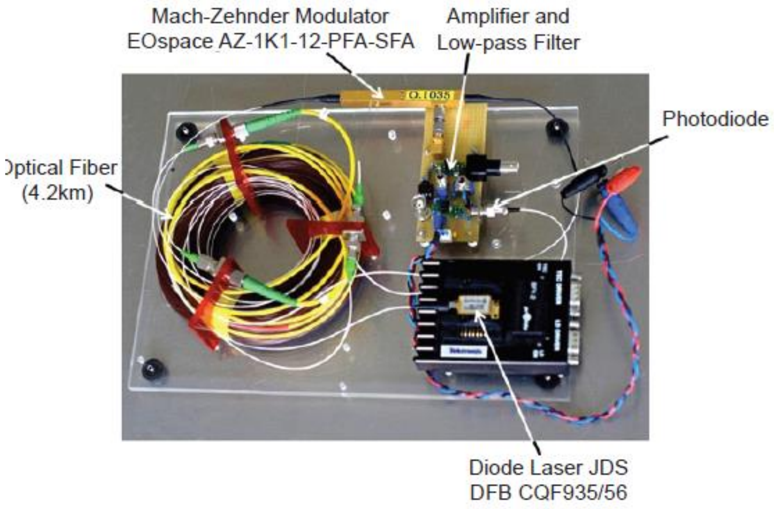
OPEN Optoelectronic Reservoir Computing

Y. Paquot[1], F. Duport[1], A. Smerieri[1], J. Dambre[2], B. Schrauwen[2], M. Haelterman[1] & S. Massar[3]

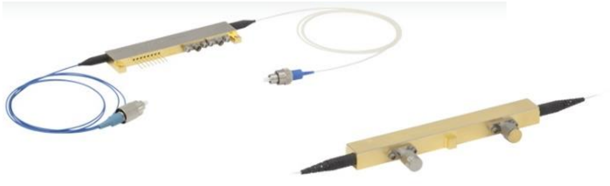
Optoelectronic Reservoir Computing

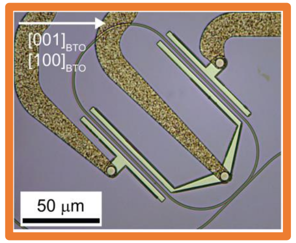




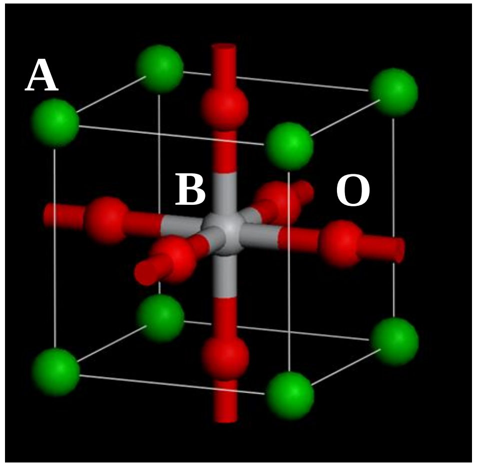


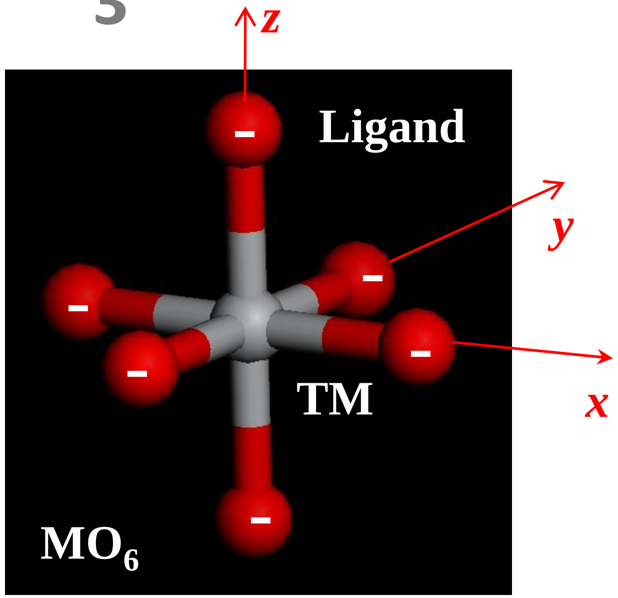
$$\varepsilon\dot{x}(s) + x(s) = \beta \sin^2\left[\mu x(s-1) + \rho u(s) + \Phi_0\right].$$





Perovskite oxides ABO_3



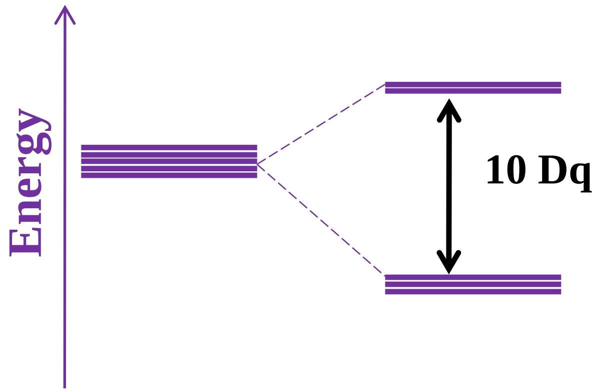


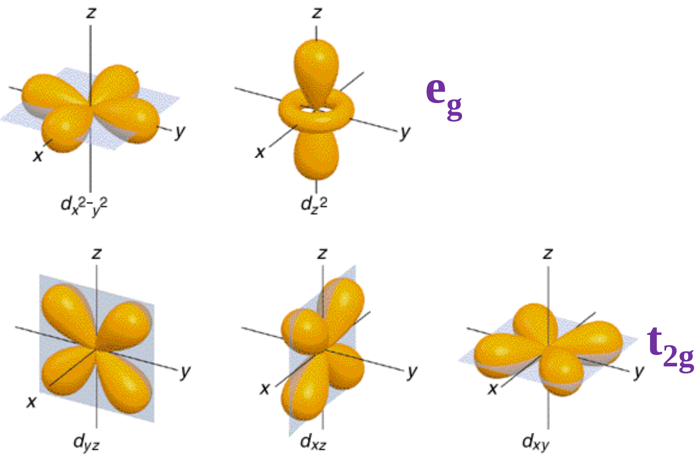
Gustav Rose
1798-1893

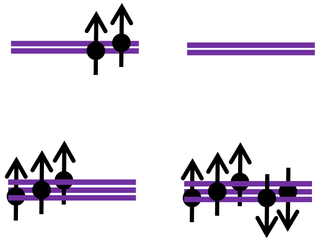
$CaTiO_3$, $BaTiO_3$, $SrHfO_3$,…

Octahedral symmetry (O_h):

High spin   Low spin
Fe^{3+} (d^5)



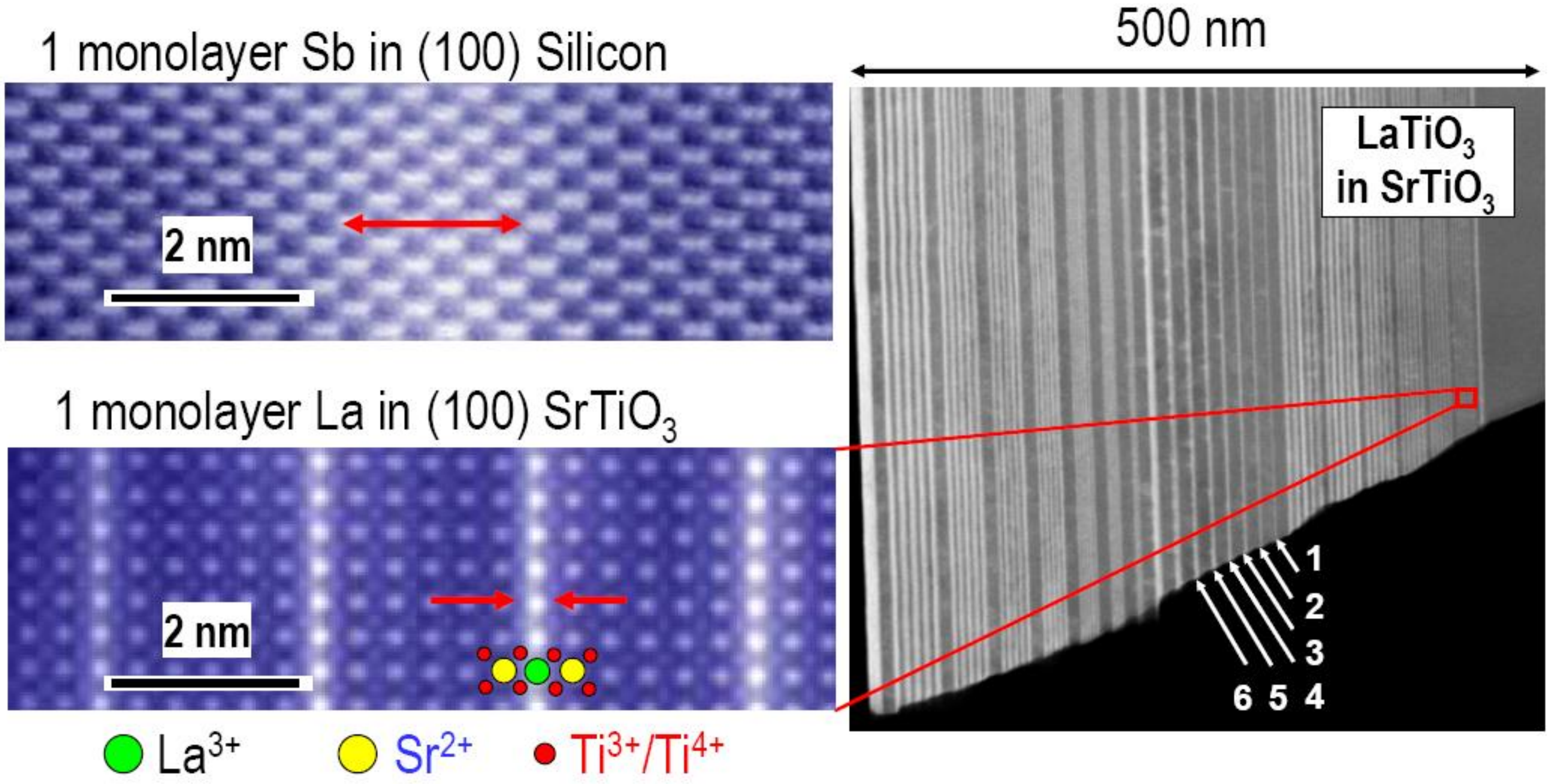




E^S-E^T=2J

Ligand field theory

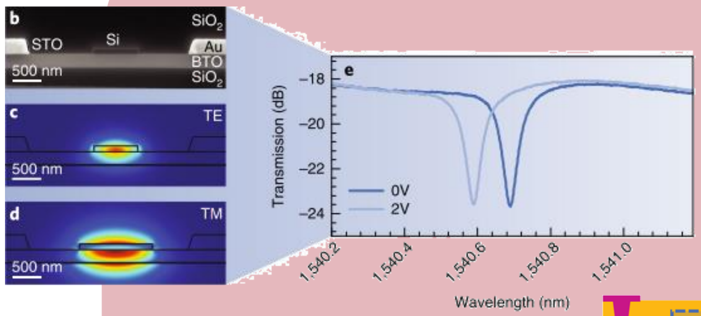
Advances in Oxide Epitaxy



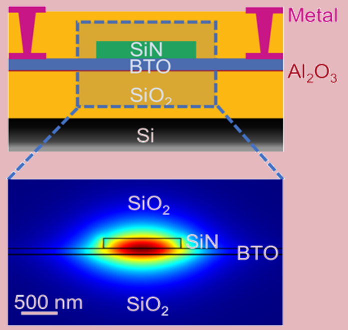
Superlattices by design

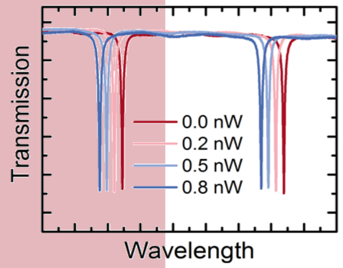
A. Ohtomo, D. A. Muller, J. A. Grazul, and H. Y. Hwang, *Nature* **419**, 378 (2002).

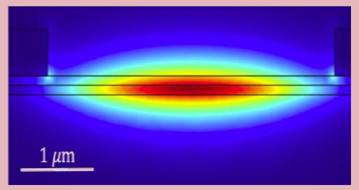
Barium Titanate Pockels Devices



- Modulators
- Switches
- Tuning elements
- Filters
- Optical memories







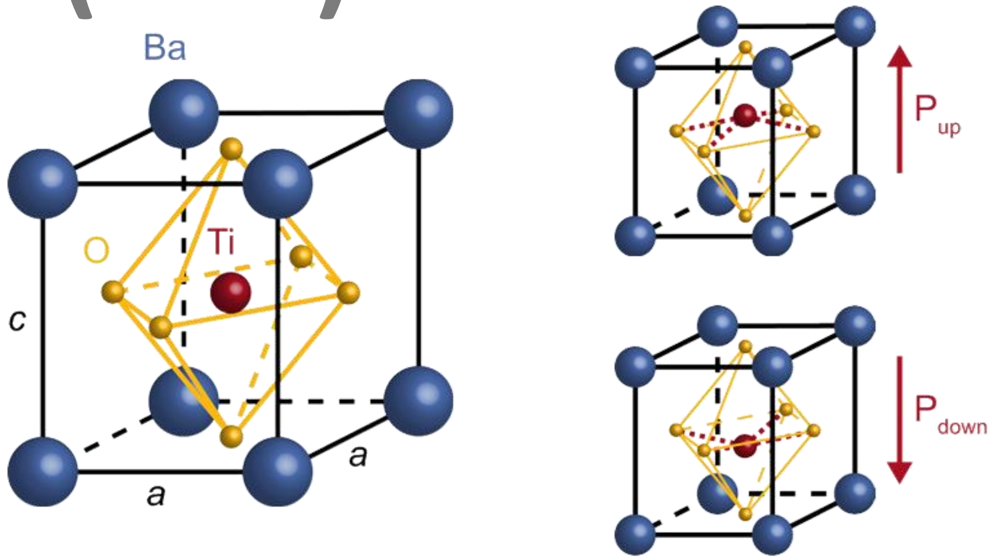
$BaTiO_3$ Barium Titanate (BTO)

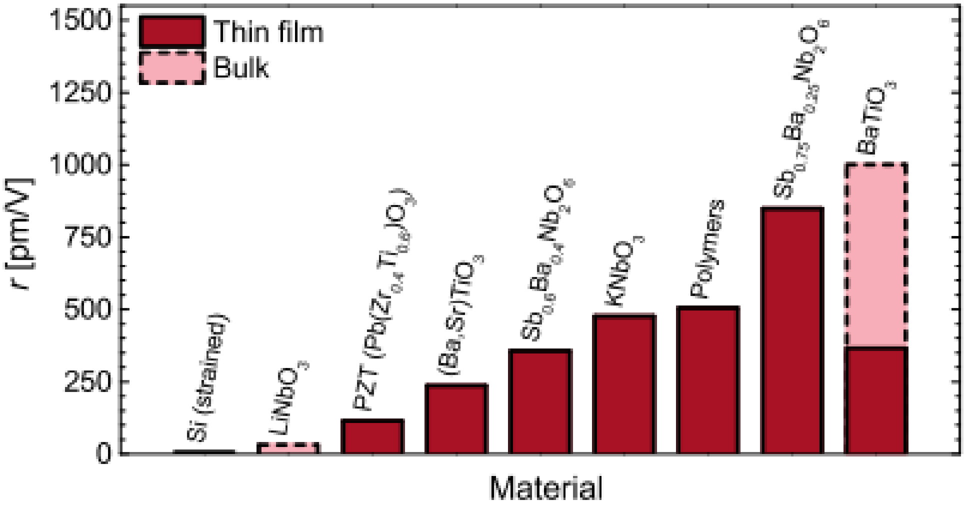
Pockels effect:

$$n(E) = n_0 - \frac{1}{2} r n_0^3 E$$

Pockels coefficient

Zero-field refractive index





Bulk BTO

- Ferroelectric perovskite
- Large Pockels coefficient

Pockels

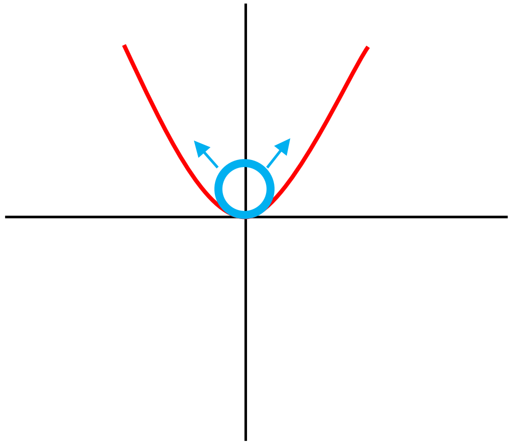
- Useful for high-speed optical modulation
- $LiNbO_3$ used in high-speed modulators
- $LiNbO_3$ incompatible with Si photonics

S. Abel, *et al.*, *Journal of Lightwave Technology* **34**, 8 (2016)

Linear Electro-optical Effect:

Anharmonic oscillator:

$$\ddot{x}+\Gamma\dot{x}+\omega_0^2 x+\nu x^2 = e/m\{E_l(\omega,t)+\beta E_{ex}(0)\}$$



Friedrich Pockels (1865–1913) was first to describe the linear electro-optic effect in 1893.

$$y = x-\frac{e\beta E_{ex}(0)}{m\omega_0^2},$$

$$y=\frac{-\frac{e}{m}Ee^{i\omega t}}{\omega_0^2-\omega^2-i\Gamma+\frac{2e\beta E_{ex}\nu}{m\omega_0^2}}-\left(\frac{e\beta E_{ex}}{m\omega_0^2}\right)^2\cdot\frac{\nu}{\omega_0^2+\frac{2e\beta E_{ex}}{m\omega_0^2}}.$$

$$\Delta n=-\frac{eN}{2n\varepsilon_0}y.$$

$$\Delta n_{Pockels}=\frac{\partial\Delta n(E_{ex}=0)}{\partial E_{ex}}E_{ex}=-\frac{eN}{2n\varepsilon_0}\cdot\frac{\partial y(E_{ex}=0)}{\partial E_{ex}}E_{ex}.$$

$$r=\frac{1}{n^4}\cdot\frac{e^3N\nu}{\varepsilon_0 m^2\omega^2}\cdot\frac{1}{(\omega_0^2-\omega^2+i\Gamma)^2}$$

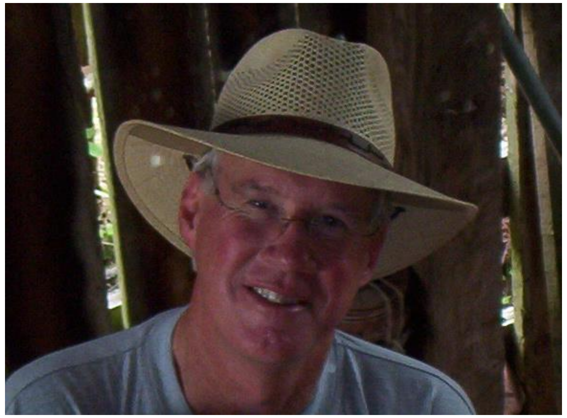
Landau-Ginzburg theory:

$$rE=\Delta\left(\frac{1}{\varepsilon}\right)\approx\frac{-\Delta\varepsilon}{\varepsilon^2}=\frac{-\chi^{(2)}E}{(1+\chi^{(1)})^2}=\frac{3\beta P(\chi^{(1)})^3E}{(1+\chi^{(1)})^2}$$

$$\chi^{(2)}=\frac{\partial^2P}{\partial E^2}=-\frac{\partial^2E}{\partial P^2}\left(\frac{\partial P}{\partial E}\right)^3=-6\beta P\left(\chi^{(1)}\right)^3$$

Anharmonic bonding, no center of inversion, and divergence of $\chi^{(1)}$

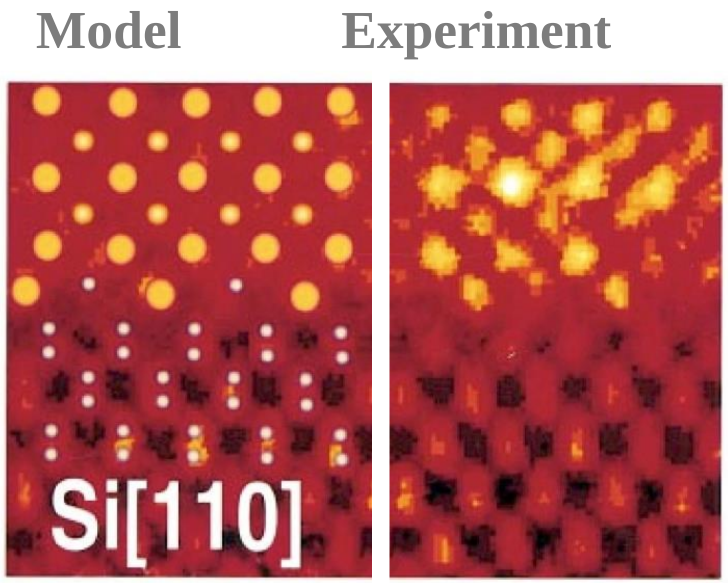
Epitaxial oxide on semiconductors

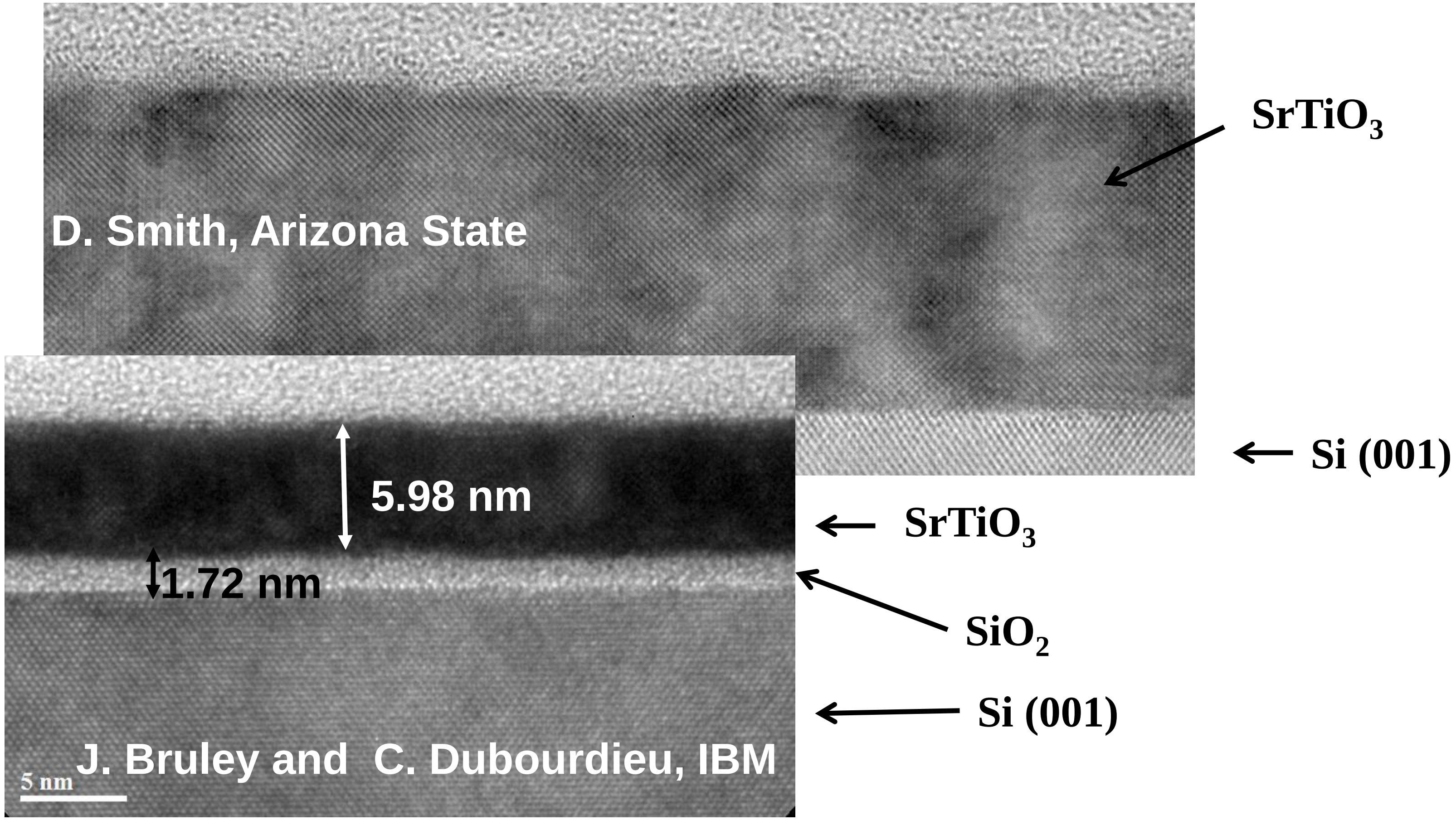


R. McKee, F. Walker, J. Conner, et al., *Appl. Phys. Lett.* 59, 782 (1991)
R. McKee, F. Walker, M. Chisholm, *Phys. Rev. Lett.* 81 3014 (1998)
R. McKee, F. Walker, M. Chisholm, *Science 293, 468 (2001)*
K. Eisenbeiser, J. Finder, Z. Yu, et al. , *Appl. Phys. Lett.* 76, 1324 (2000)
C. Dubourdieu, J. Bruley, T. M. Arruda, et al., Nature Nanotechnology 8, 748 (2013).

A. A. Demkov and A. B. Posadas, *Integration of Functional Oxides with Semiconductors*, (Springer, 2014)
L. Mazet, et al. , Sci. Technol. Adv. Mater. 16 036005 (2015)

$SrTiO_3$ on Si

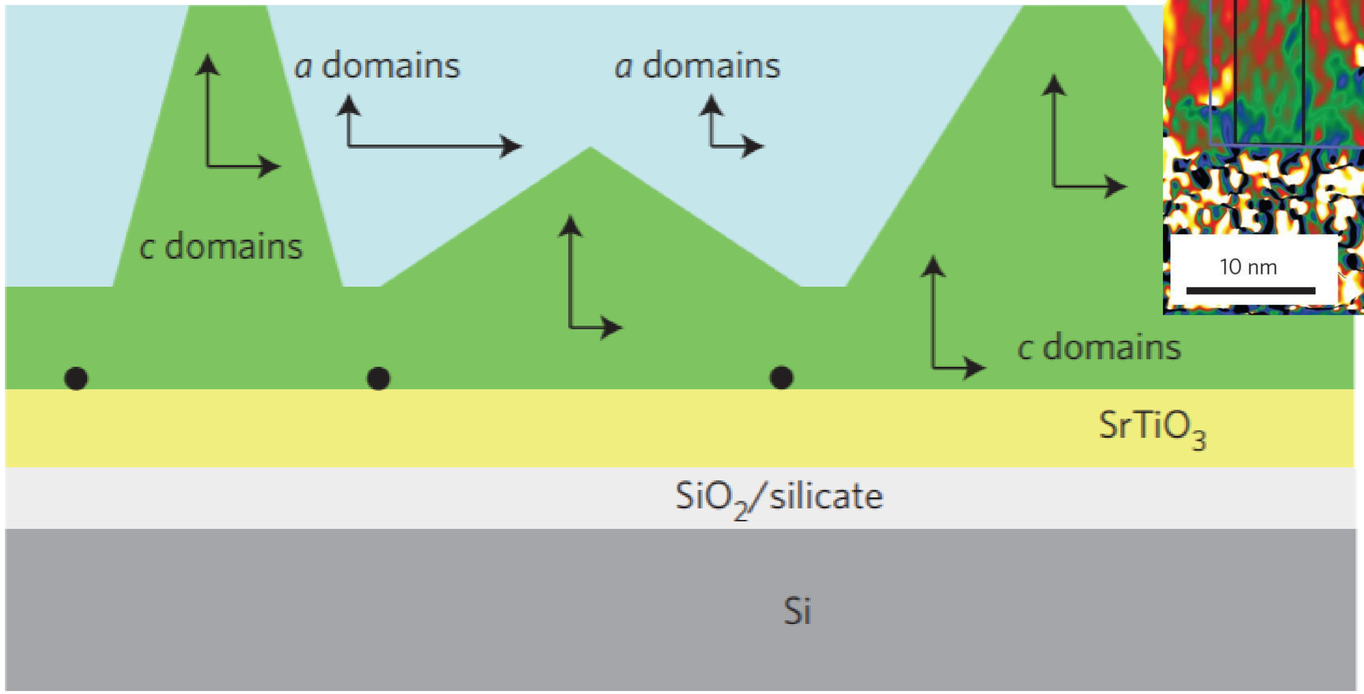


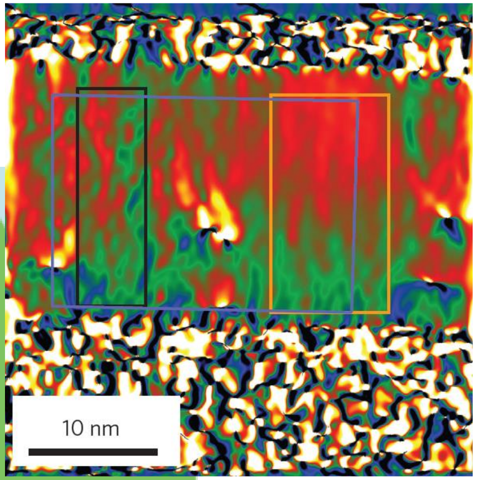


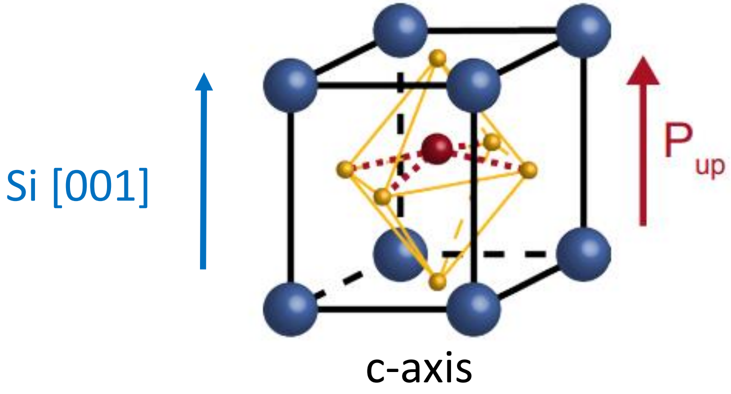
a-axis vs c-axis oriented $BaTiO_3$ on Si

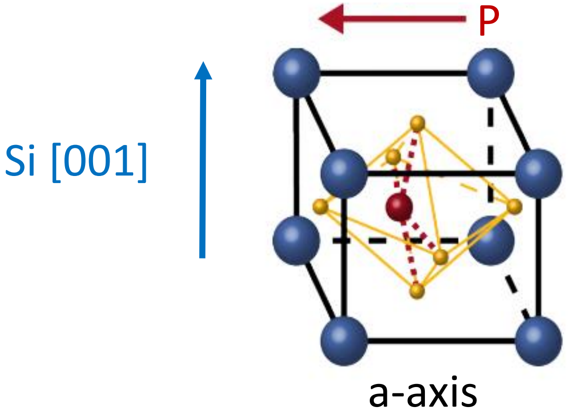
- Initially BTO grows oriented c-axis
- As film thickness increases(≳ 50 nm), BTO relaxes and forms some a-axis domains
- Is it possible to reorient the c-axis to a-axis in ≲ 50 nm films?

Dubourdieu et. al, Nature Nanotechnology 8.10 748 (2013)

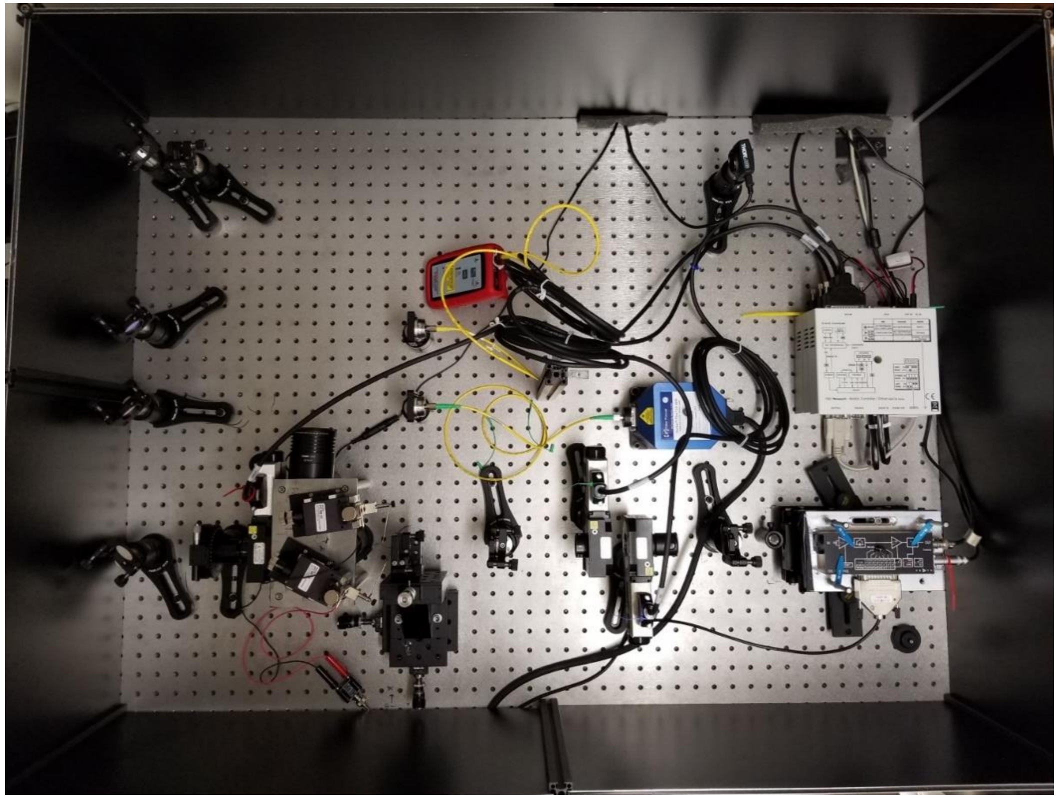


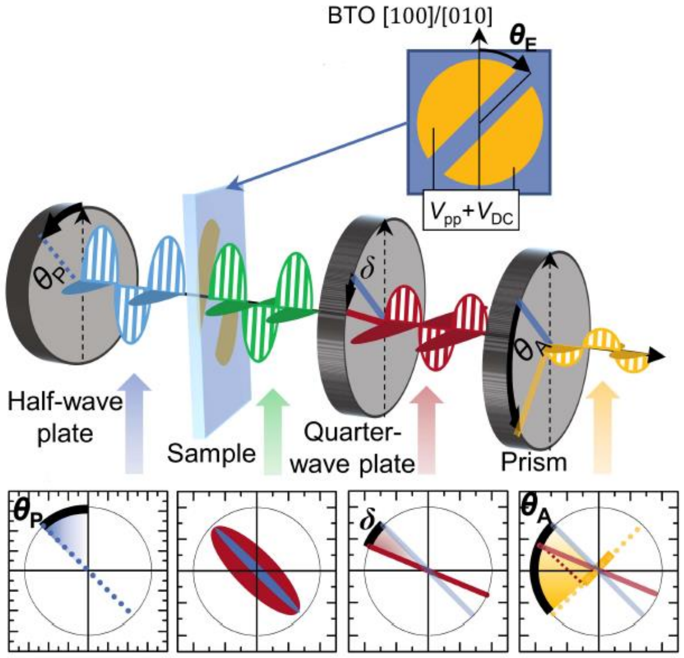


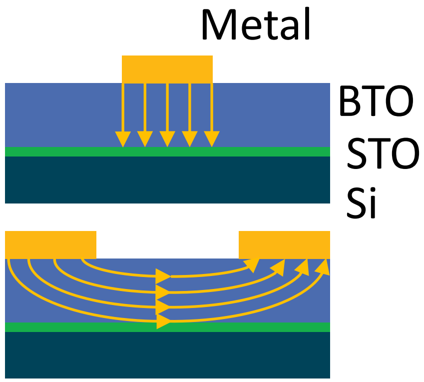




Measuring Pockels effect in thin films







$$P_{DC} = P_0 cos^2(\theta_a)$$

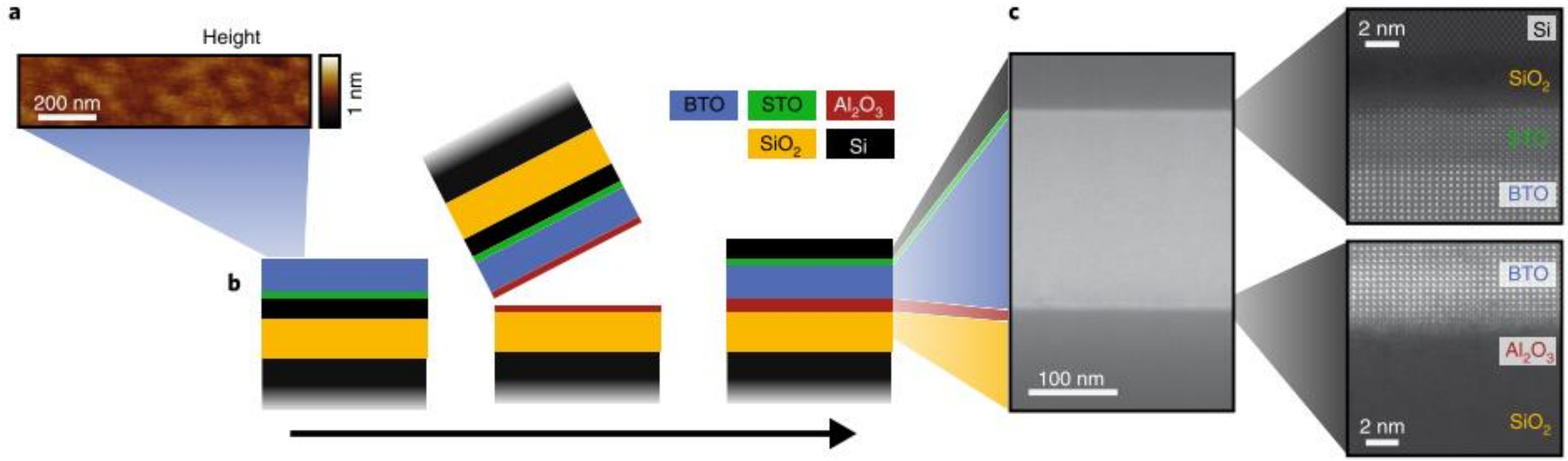
$$P_{DC\delta} = P_0 cos^2(\theta_a + \delta)$$

$$P_{DC} - P_{DC\delta} \approx dP \; for \; small \; \delta$$

S. Abel, T. Stöferle, C. Marchiori, C. Rossel, M.D. Rossell, R. Erni, D. Caimi, M. Sousa, A. Chelnokov, B.J. Offrein, and J. Fompeyrine, Nat. Commun. **4**, 1671 (2013).

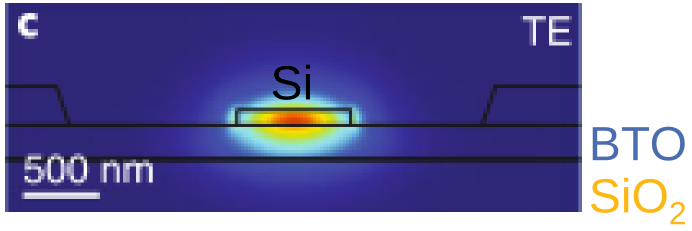
K.J. Kormondy *et al.*, Nanotechnol. **28** (2017)

Hybrid BTO-Si Devices



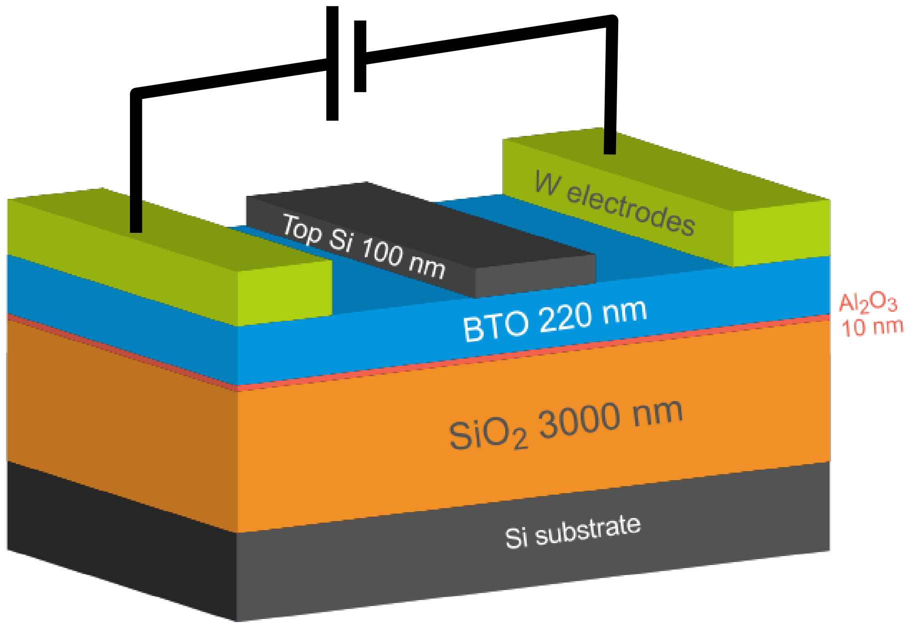
Device Structure

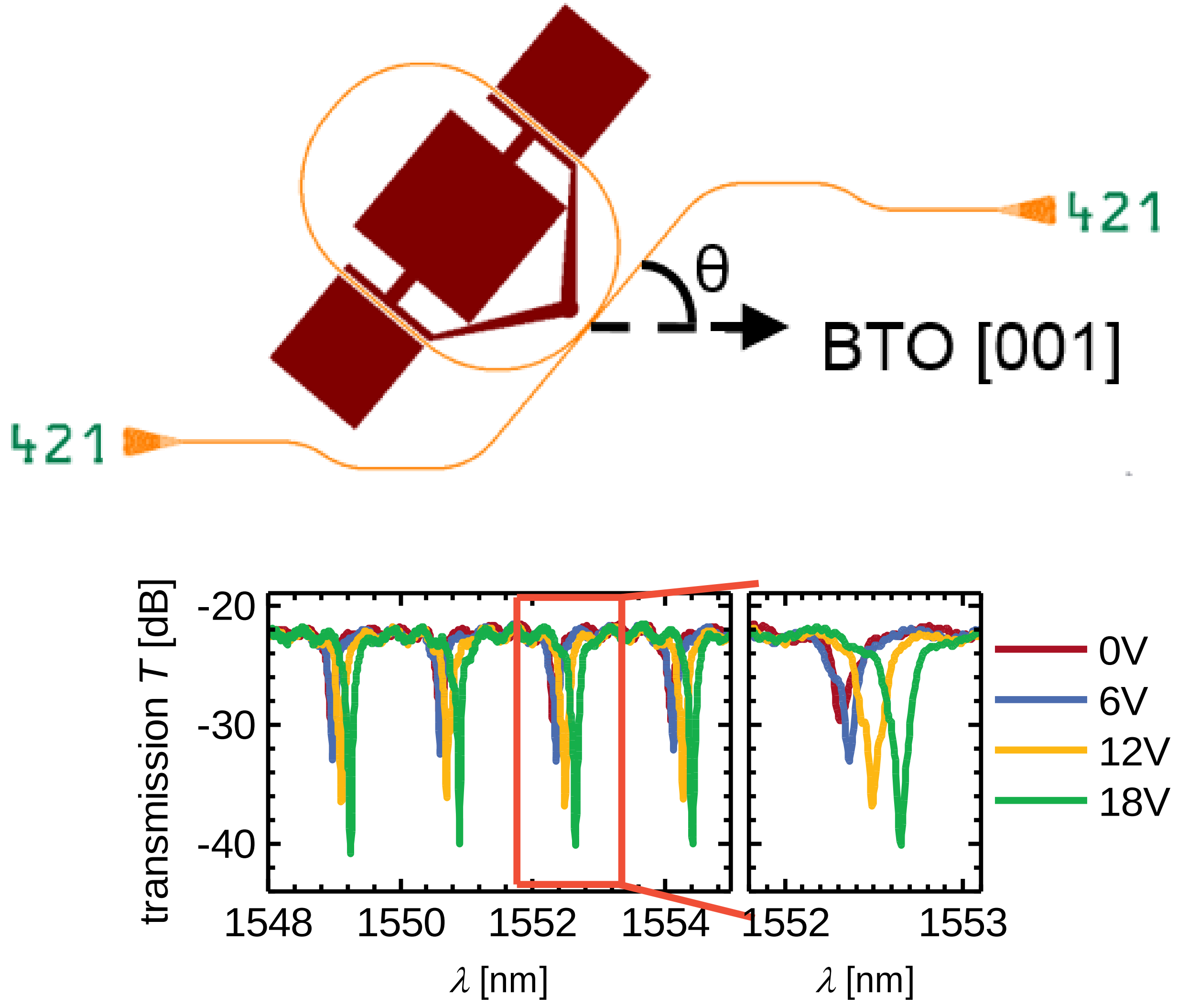
- Si strip waveguide on BTO
- Bonded to SiO_2
- Offers better electrical and optical isolation than SOI



Abel, Eltes, Ortmann, *et al.*, *Nature Mat.* **18**, 42 (2019)

Active Devices: Racetrack Resonators





Abel *et al.*, Journal of Lightwave Technology

Device design

- Resonant device
- Well-defined electric field angle
- Resonance wavelength according to:

$$m * \lambda_m = d * n_{eff}$$

m: Order number

λ_m: Resonance wavelength

$d * n_{eff}$: Optical path length

Optical Resonator Basics

Resonators for Pockels Characterization

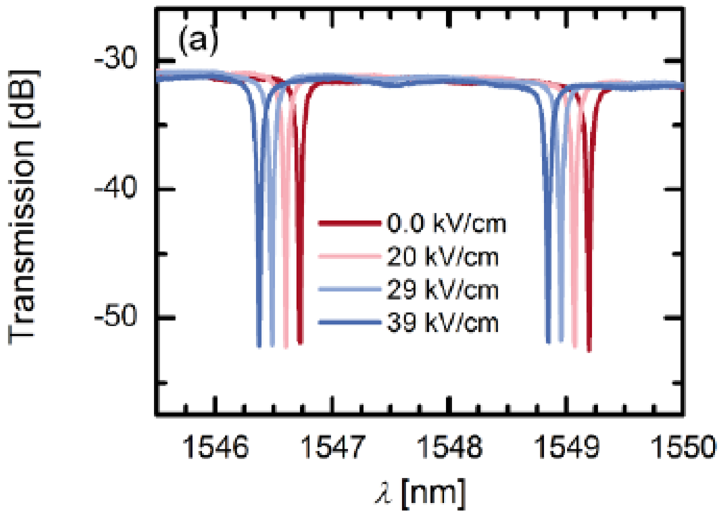
- Well-defined electric field angle
- Resonance wavelength according to:

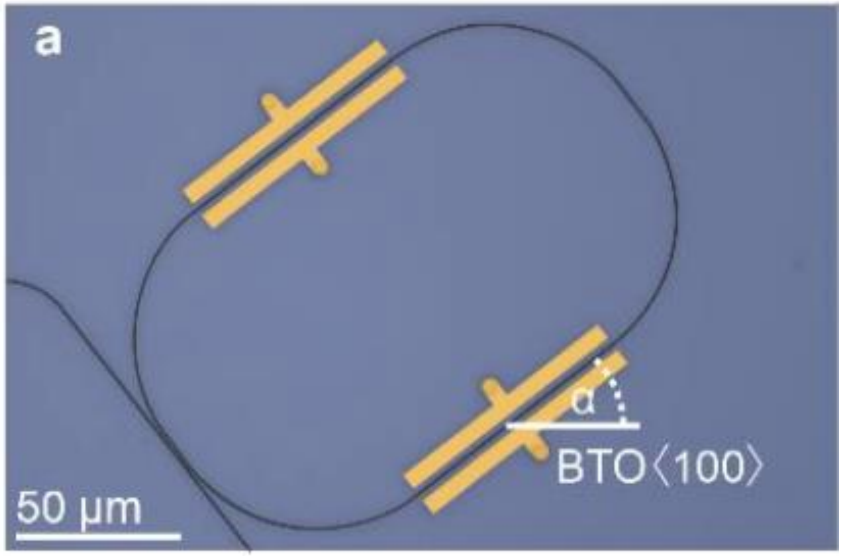
$$m * \lambda_m = d * n$$

Order number

Resonance wavelength

Optical path length



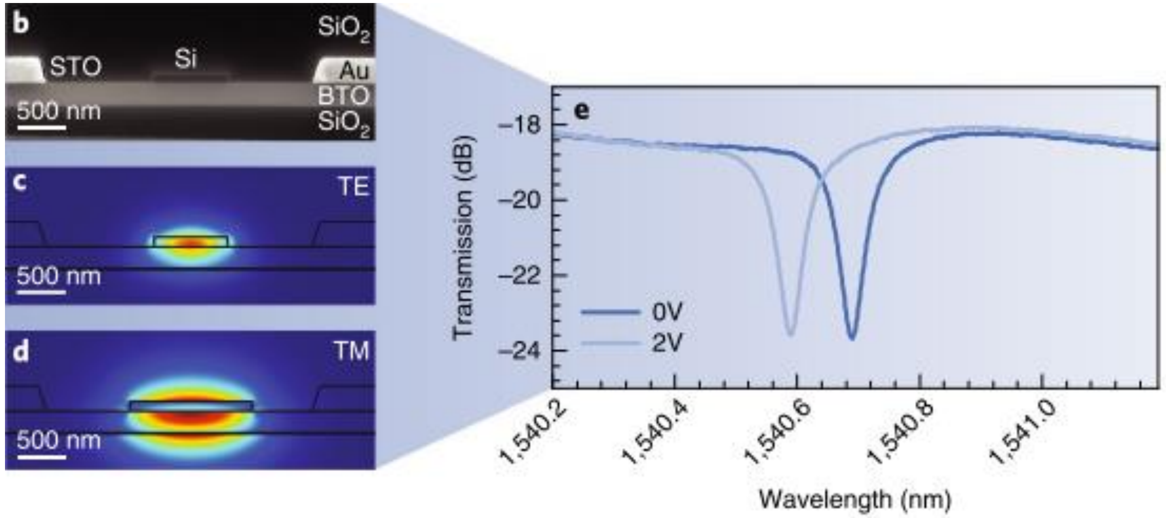


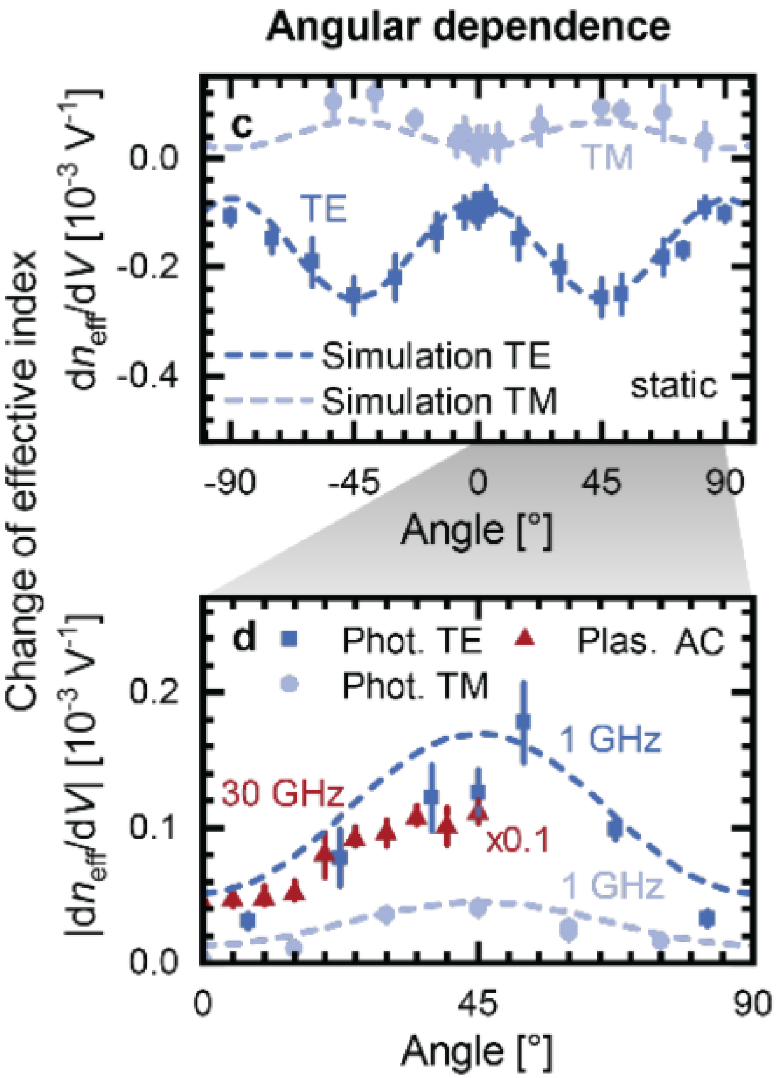
Recall:

$$n(E) = n_0 - \frac{1}{2} r n_0^3 E$$

Abel, Eltes, Ortmann, *et al.*, *Nature Mat.* **18**, 42 (2019)

Pockels Effect in Hybrid BTO-Si Devices





Proof of Pockels Effect

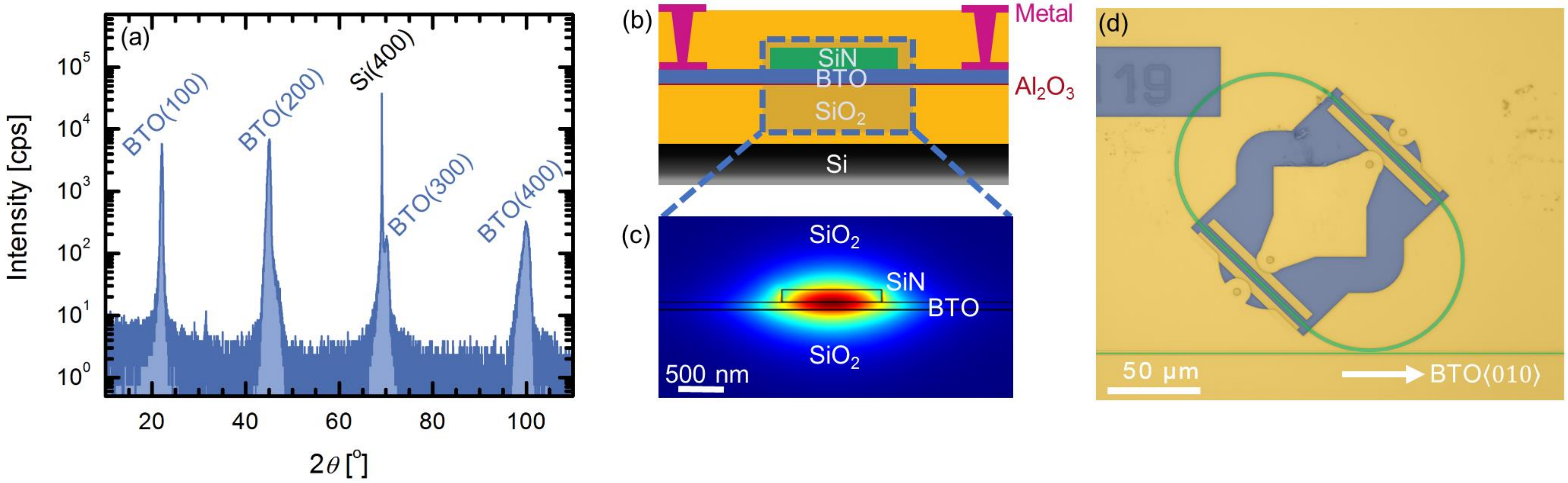
- Tracked index shift through resonance shift
- Electro-optic response shows expected anisotropies

Electro-Optic Response

- Pockels tensor element r_{51} = **923 pm/V**
- Record high response in thin films

Abel, Eltes, Ortmann, *et al.*, *Nature Mat.* **18**, 42 (2019)

Hybrid BTO-SiN Devices



Device Structure

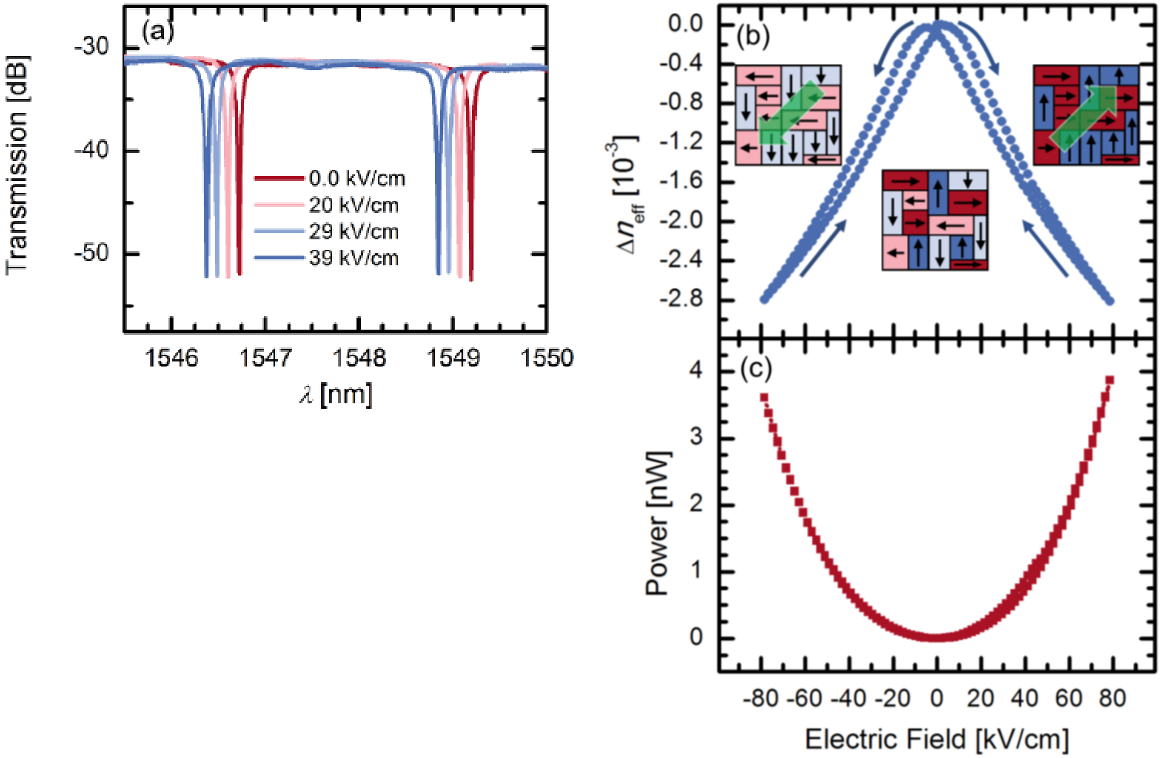
- Replace with insulating silicon nitride

Photonics

- Devices support single TE mode
- Fabricated resonant structures

Ortmann, *et al.*, "Ultra-Low Power Tuning in Hybrid Barium Titanate-Silicon Nitride Electro-Optic Devices on Silicon", **ACS Photonics** (2019)

Device Tuning



Resonances

- Sharp resonances
- Tuned with electric field
- No extinction ratio change even at high bias
- Ferroelectric hysteresis

Power Consumption

- Very low leakage leads to very small power consumption

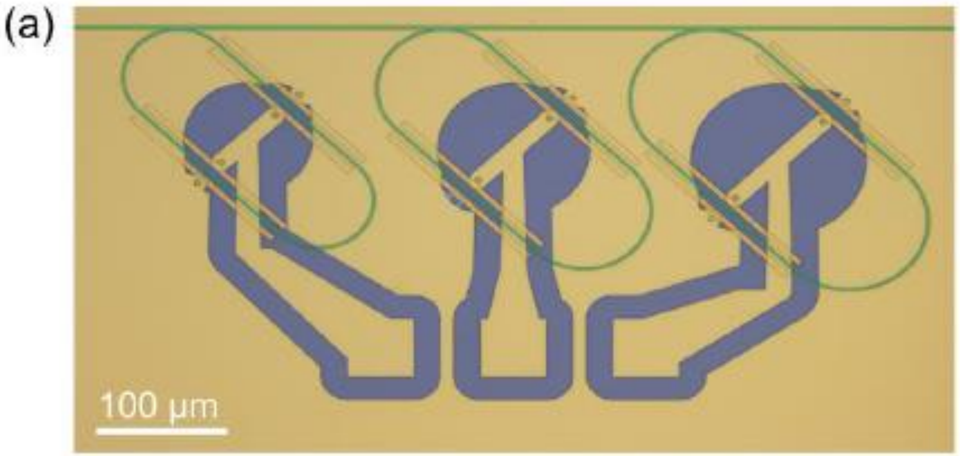
Table 1: Power consumption comparison between electro-optic devices compatible with standard PIC integration routes, exploiting different tuning mechanisms

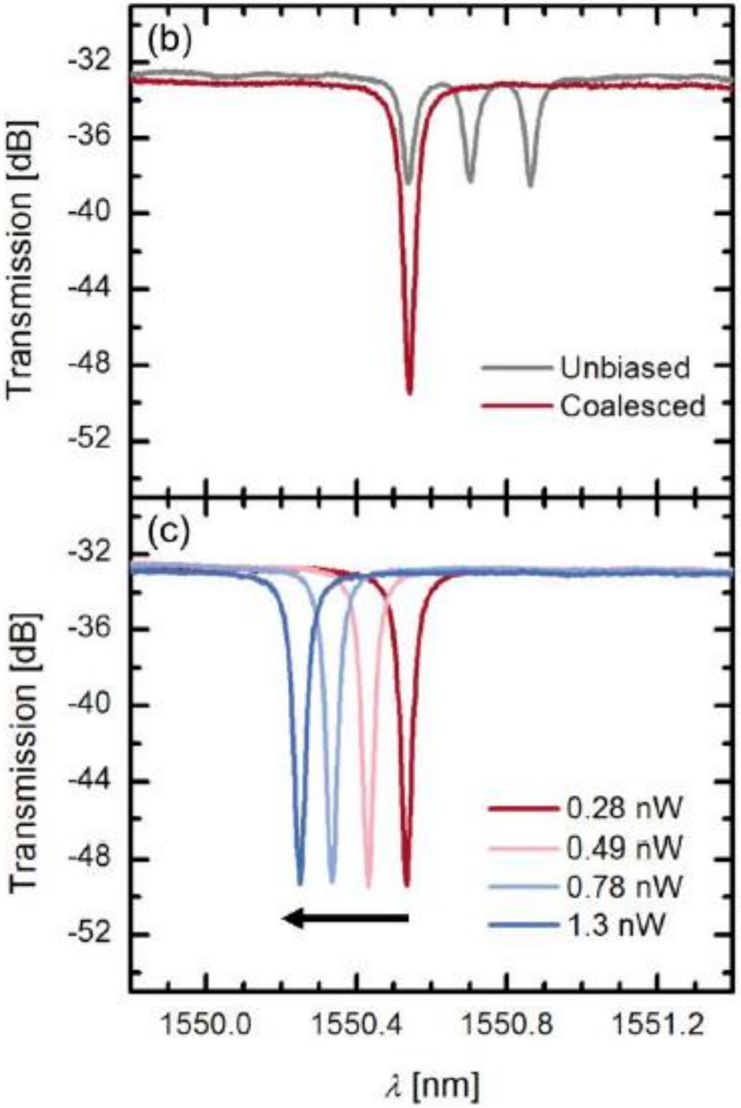
tuning mechanism	reference	power consumption (μW/FSR)
Thermo-optic	Atabaki *et al.*[29]	24500
Thermo-optic	Dong *et al.*[44]	21000
Thermo-optic	Dong *et al.*[28]	2400
Plasma dispersion in Si[a]	Timurdogan *et al.*[27]	>500
Pockels effect	Abel *et al.*[41]	4
Pockels effect	This work	0.106

[a] Power consumption extrapolated from tuning data presented in Timurdogan *et al.*

Ortmann, *et al.*, "Ultra-Low Power Tuning in Hybrid Barium Titanate-Silicon Nitride Electro-Optic Devices on Silicon", **ACS Photonics**(2019)

Multi-Resonator Filters





Tunable Filters

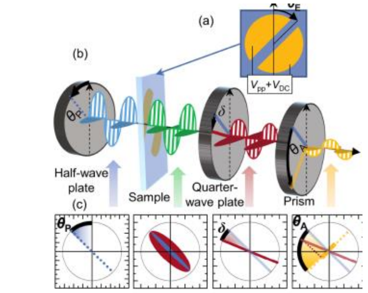
- Can design tunable filter in BTO-based devices
  - Compensate fab tolerances
- Multi-resonator allows for potentially very deep extinction ratios

Performance

- Can coalesce individual resonances
- Coalesced resonance can be further tuned

Ortmann, *et al.*, "Ultra-Low Power Tuning in Hybrid Barium Titanate-Silicon Nitride Electro-Optic Devices on Silicon", **ACS Photonics**(2019)

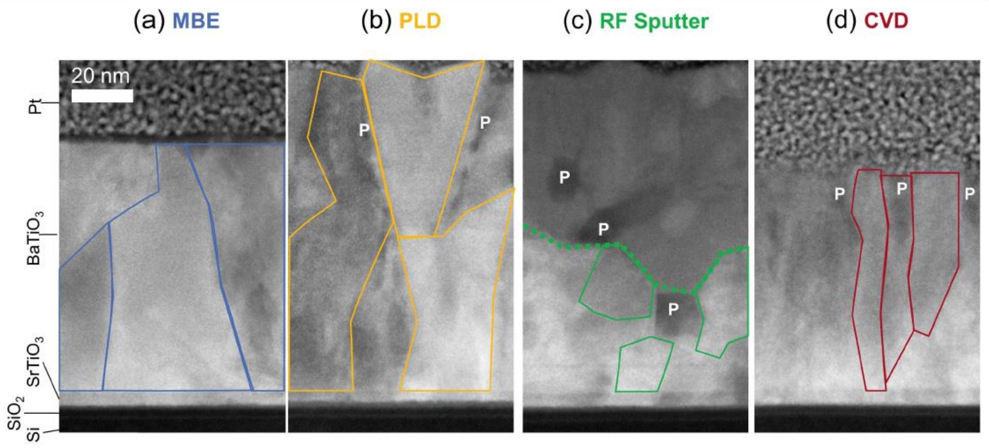
Integrated Ferroelectric Perovskites Can be used in Si photonics

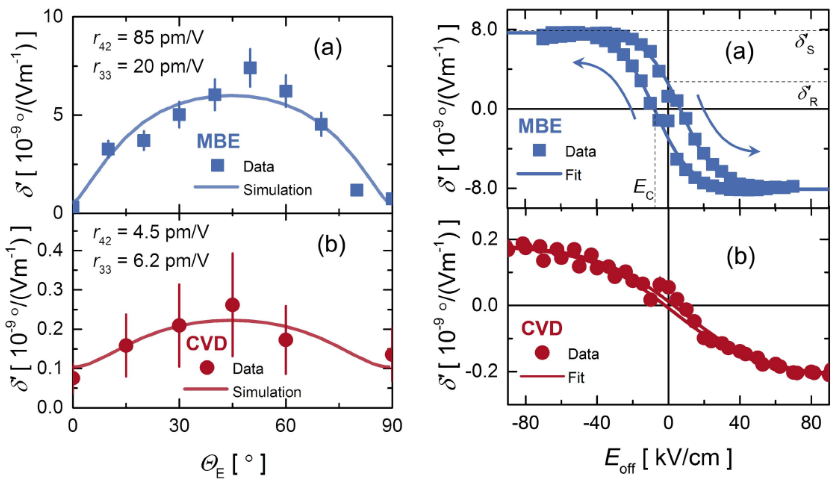


IOP Publishing Nanotechnology
Nanotechnology 28 (2017) 075706 (10pp) doi:10.1088/1361-6528/aa53c2

Microstructure and ferroelectricity of $BaTiO_3$ thin films on Si for integrated photonics

Kristy J Kormondy[1], Youri Popoff[2], Marilyne Sousa[2], Felix Eltes[2], Daniele Caimi[2], Marta D Rossell[3], Manfred Fiebig[4], Patrik Hoffmann[5,6], Chiara Marchiori[2], Michael Reinke[5,6], Morgan Trassin[4], Alexander A Demkov[1], Jean Fompeyrine[2] and Stefan Abel[2]

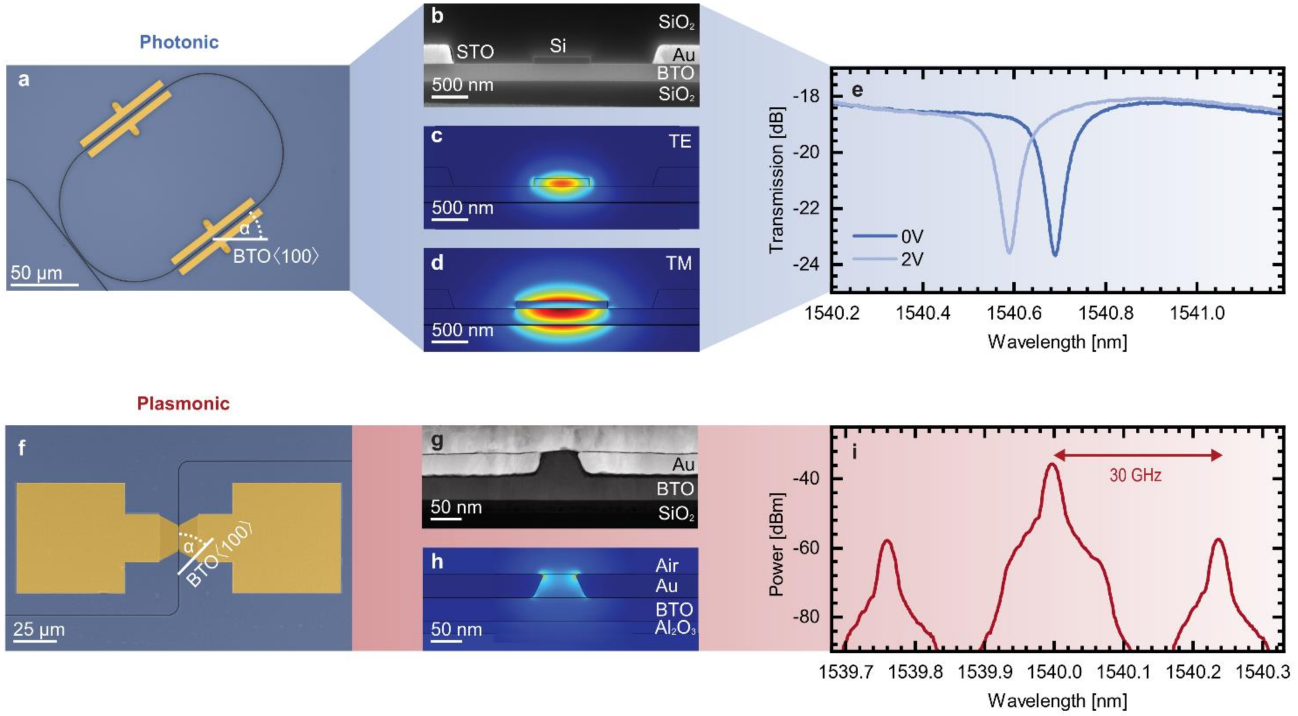




DispatchDate: 09.10.2018 · ProofNo: 208, p.1
nature materials ARTICLES
https://doi.org/10.1038/s41563-018-0208-0

Large Pockels effect in micro- and nanostructured barium titanate integrated on silicon

Stefan Abel[1,7]*, Felix Eltes[1,7], J. Elliott Ortmann[2], Andreas Messner[3], Pau Castera[4], Tino Wagner[5], Darius Urbonas[1], Alvaro Rosa[4], Ana M. Gutierrez[4], Domenico Tulli[6], Ping Ma[3]*, Benedikt Baeuerle[3], Arne Josten[3], Wolfgang Heni[3], Daniele Caimi[1], Lukas Czornomaz[1], Alexander A. Demkov[2], Juerg Leuthold[3], Pablo Sanchis[4]* and Jean Fompeyrine[1]



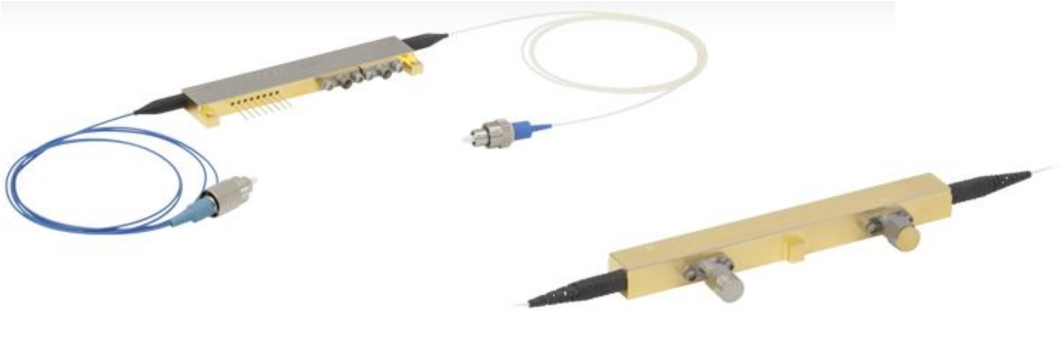
Conclusions

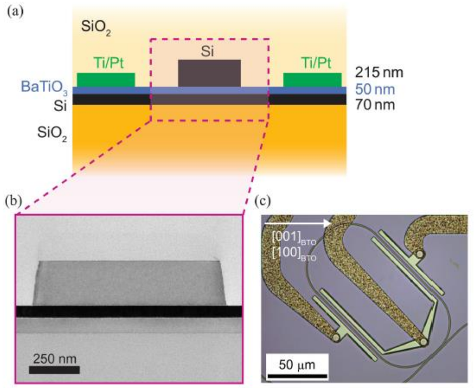
Friedrich Pockels (1865–1913) was first to describe the linear electro-optic effect in 1893.

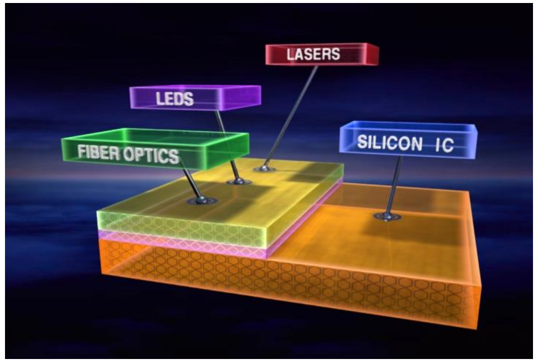
Discovery of growth methods that allow for integrating TMOs directly on Si, created revolutionary opportunities in silicon Photonics.

Such integration of highly electro-optically active films with silicon chips paves the way towards power-efficient, ultra-compact integrated devices, such as interconnects, modulators, tuning elements and bi-stable switches, all of which have defense applications.

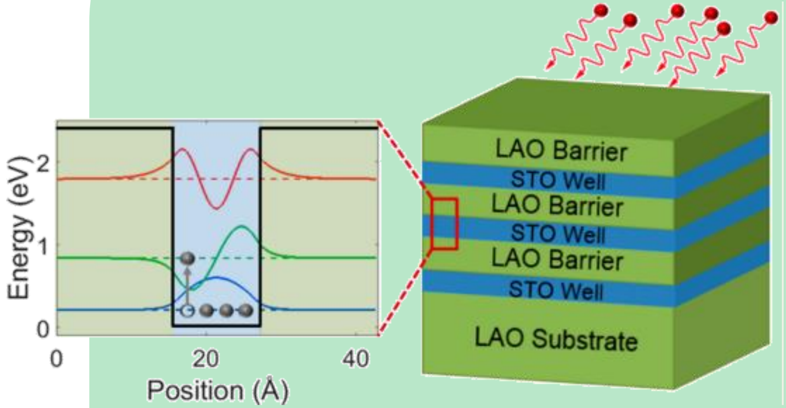
The effective EO coefficient of BTO films is twenty five times that of the current industry standard $LiNbO_3$ but is still five times lower the bulk value, the search for super-NL oxides is on!

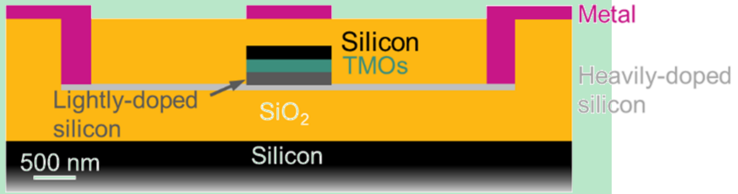




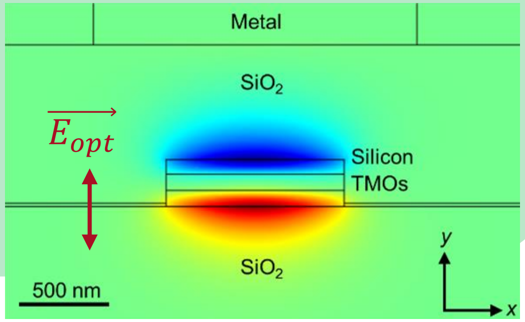


Transition Metal Oxide Quantum Wells

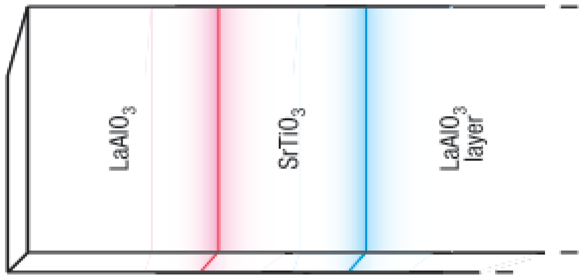


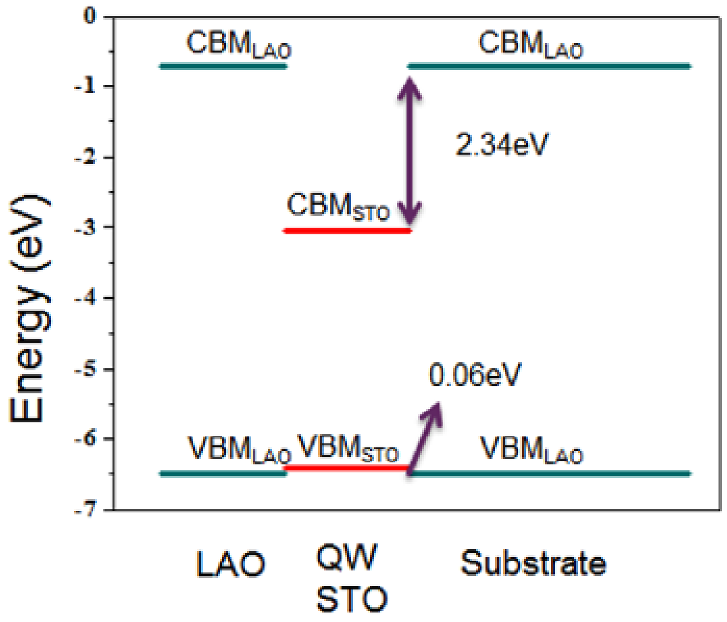


- Light sources
- Detectors
- Modulators
- Switches
- Filters



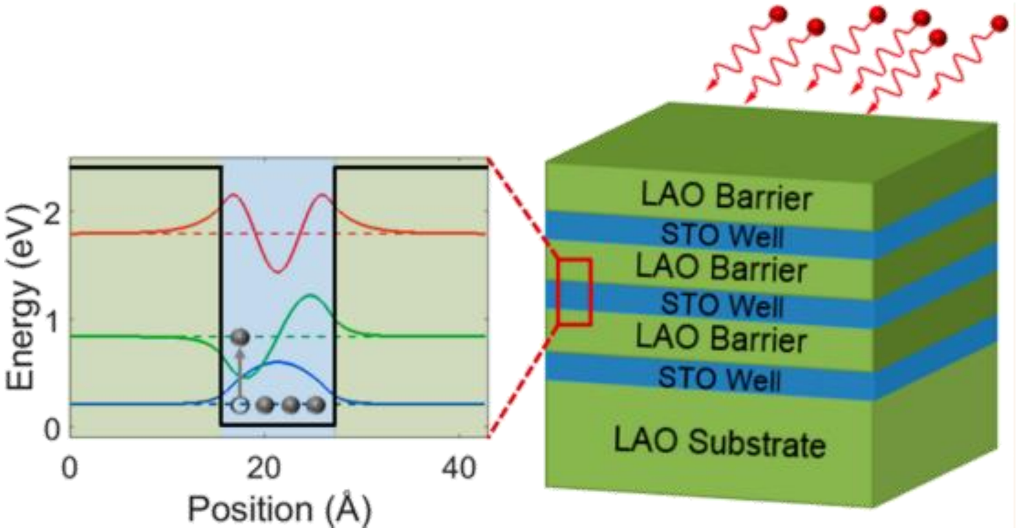
$SrTiO_3/LaAlO_3$ as a Quantum Well





Band Alignment

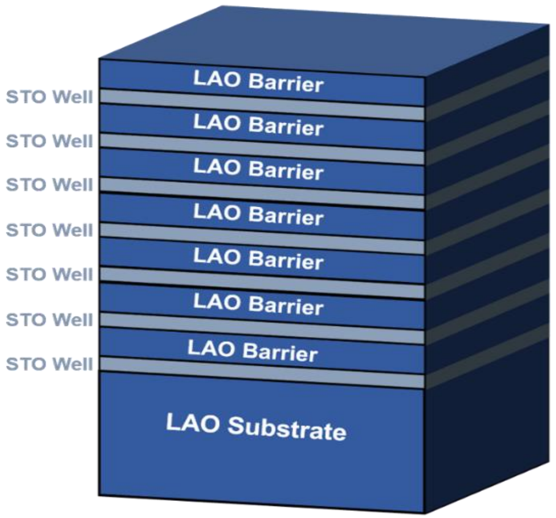
- Huge conduction band offset ~2.34 eV
  - GaAs offset ~ 0.5 eV
  - Suggests possibility of high-energy intersubband transitions



Huijben, *et al.*, *Nature Materials* **5**, 556 (2006)
Choi, *et al.*, *Appl. Phys. Lett.* **106**, 192902 (2015)
Ortmann, *et al.*, *ACS Nano* **12**, 7682 (2018)

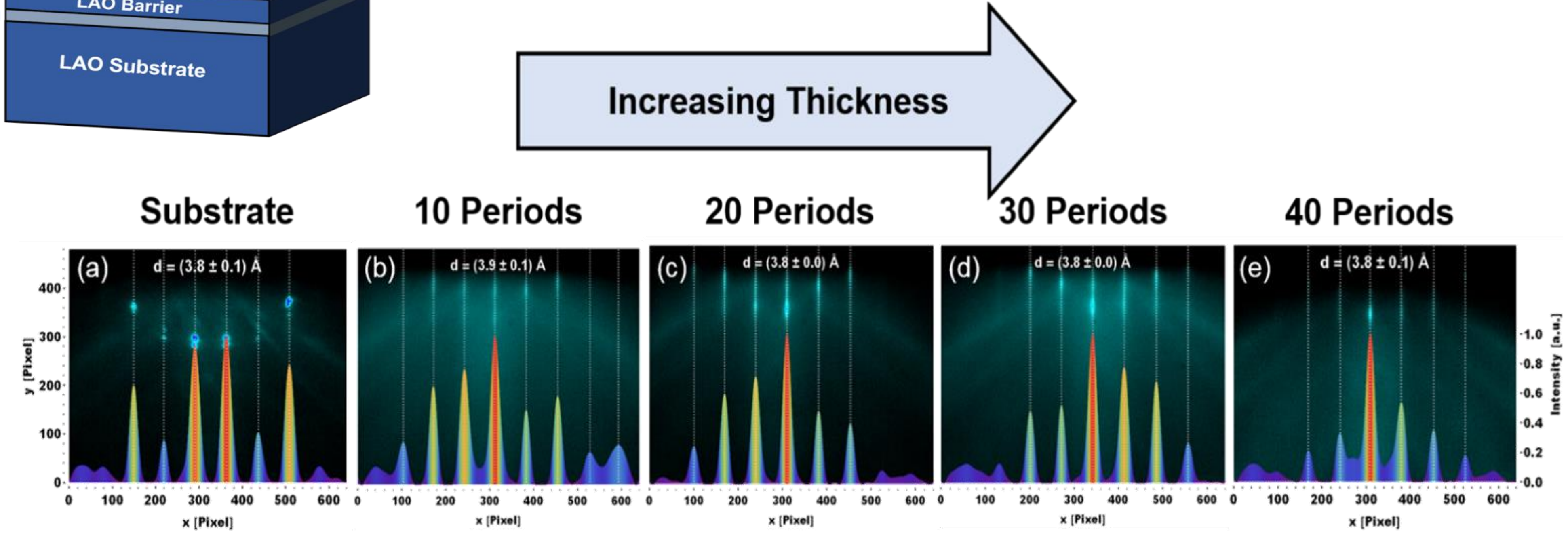
THE UNIVERSITY OF TEXAS AT AUSTIN
MaterialsPhysicsLab
DEPARTMENT OF PHYSICS

Quality Independent of Thickness



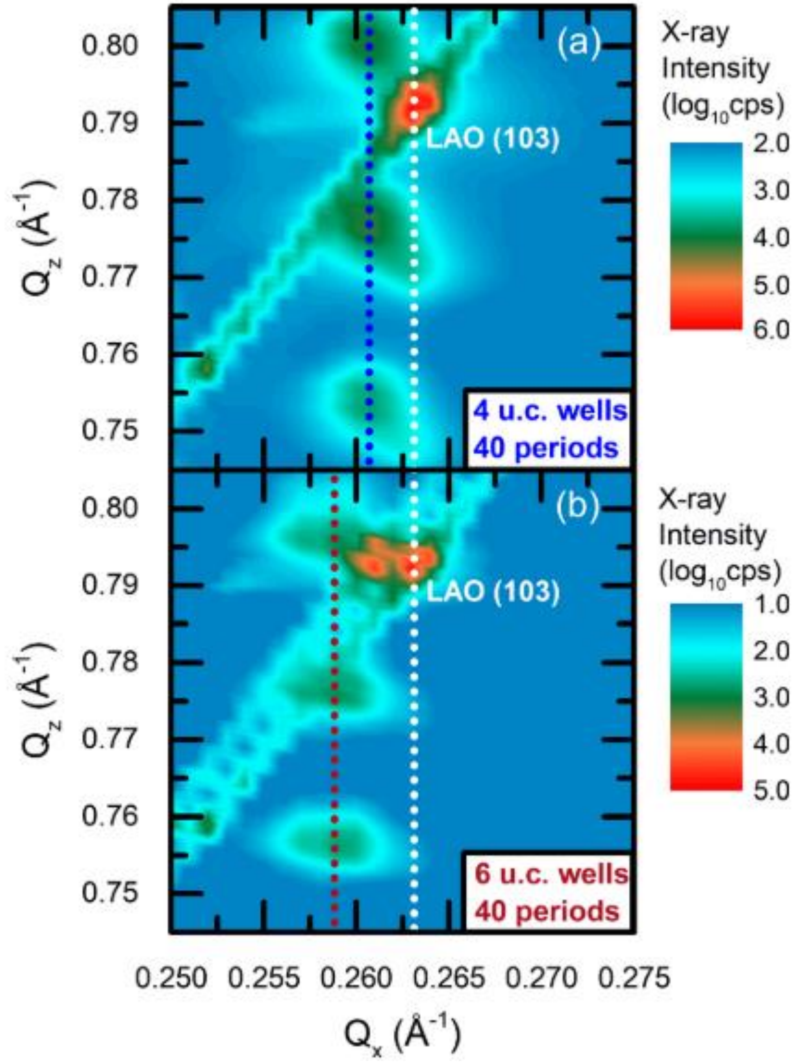
Surface Quality

- RHEED shows surface quality independent of sample thickness
- Consistent lattice constant
- Good surface quality crucial for growth of thick heterostructures



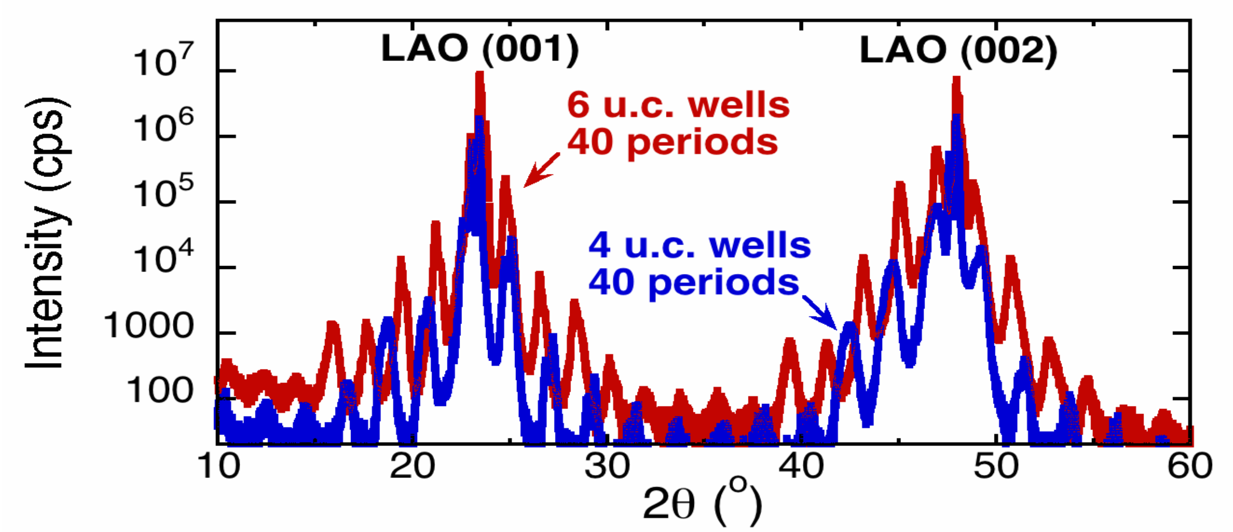
Ortmann, *et al.*, *JAP* **124**, 015301 (2018)

Quality Independent of Thickness



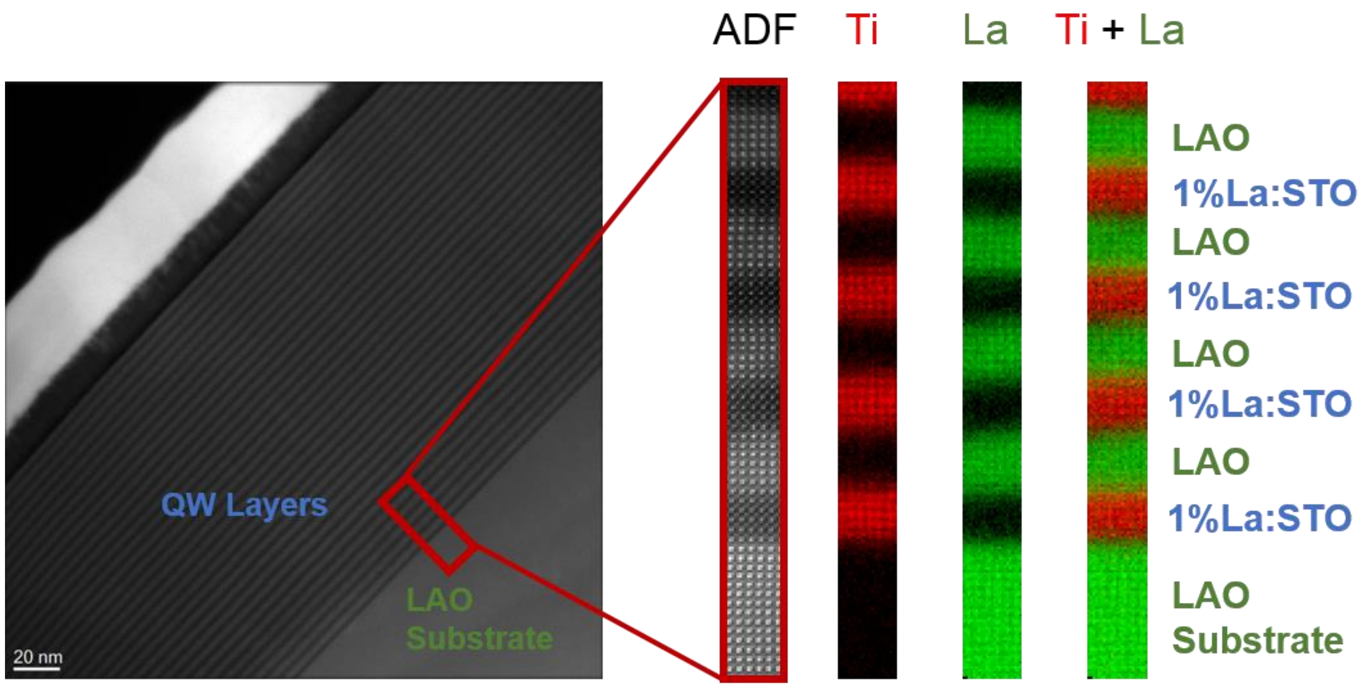
Reciprocal Space

- Clear superlattice peaks in out-of-plane direction
- Slight lattice relaxation for wider wells
- Period length constant



Ortmann, *et al.*, *JAP* **124**, 015301 (2018)

STEM of Thick Heterostructures

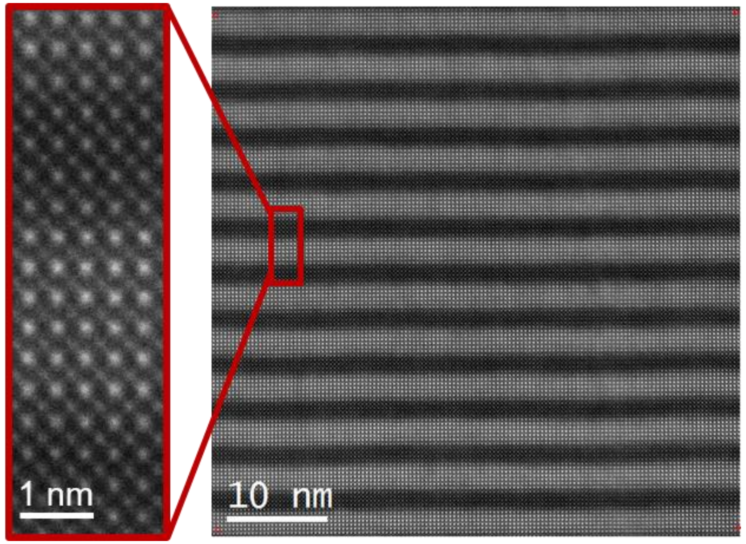


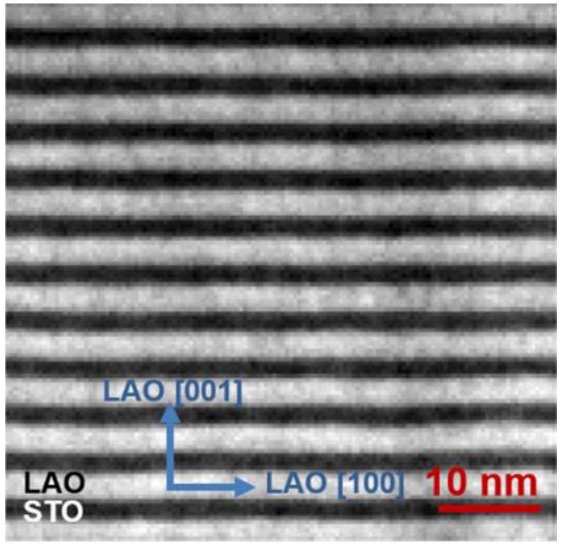
Quality

- STEM shows clear separation between STO wells and LAO barriers
- EELS mapping shows chemical modulation along growth direction
- EELS cannot detect 1at% La doping

Ortmann, *et al.*, *ACS Nano* **12**, 7682 (2018)

Statistical Analysis of Interfaces



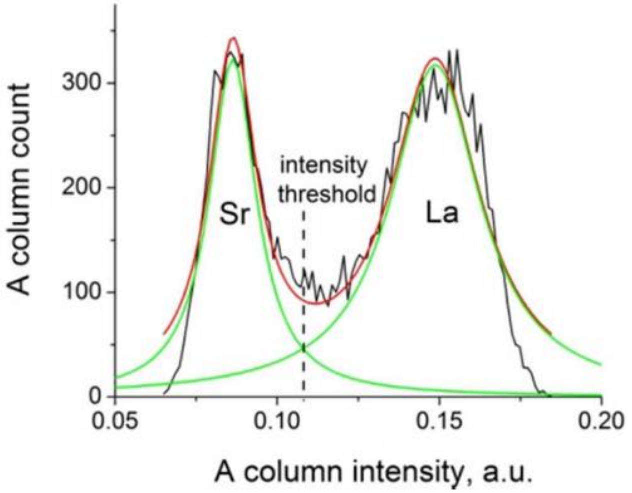


Interfacial Roughness

- Previous reports had high interfacial roughness
- Use STEM to characterize interfaces

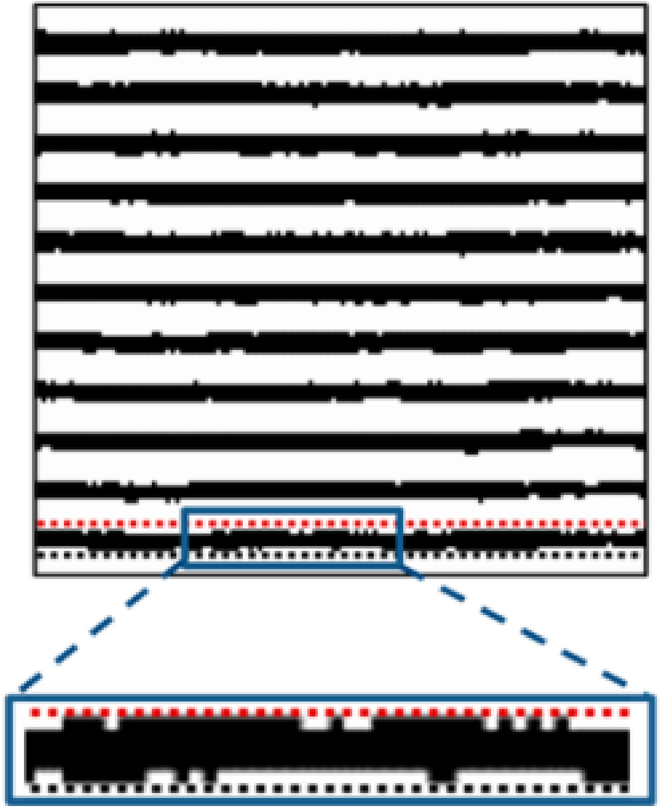
Method

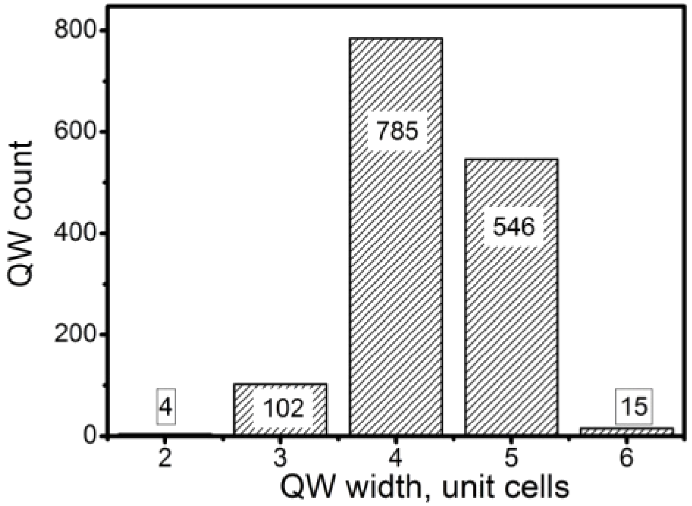
- Image sample with STEM
- Make map of *A*-site intensities
- Fit intensity to define threshold between STO and LAO unit cells



Ortmann, *et al.*, *ACS Nano* **12**, 7682 (2018)

Statistical Analysis of Interfaces

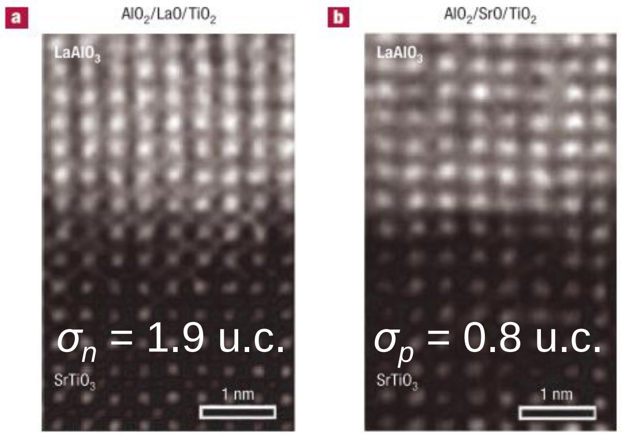




Well Sizes

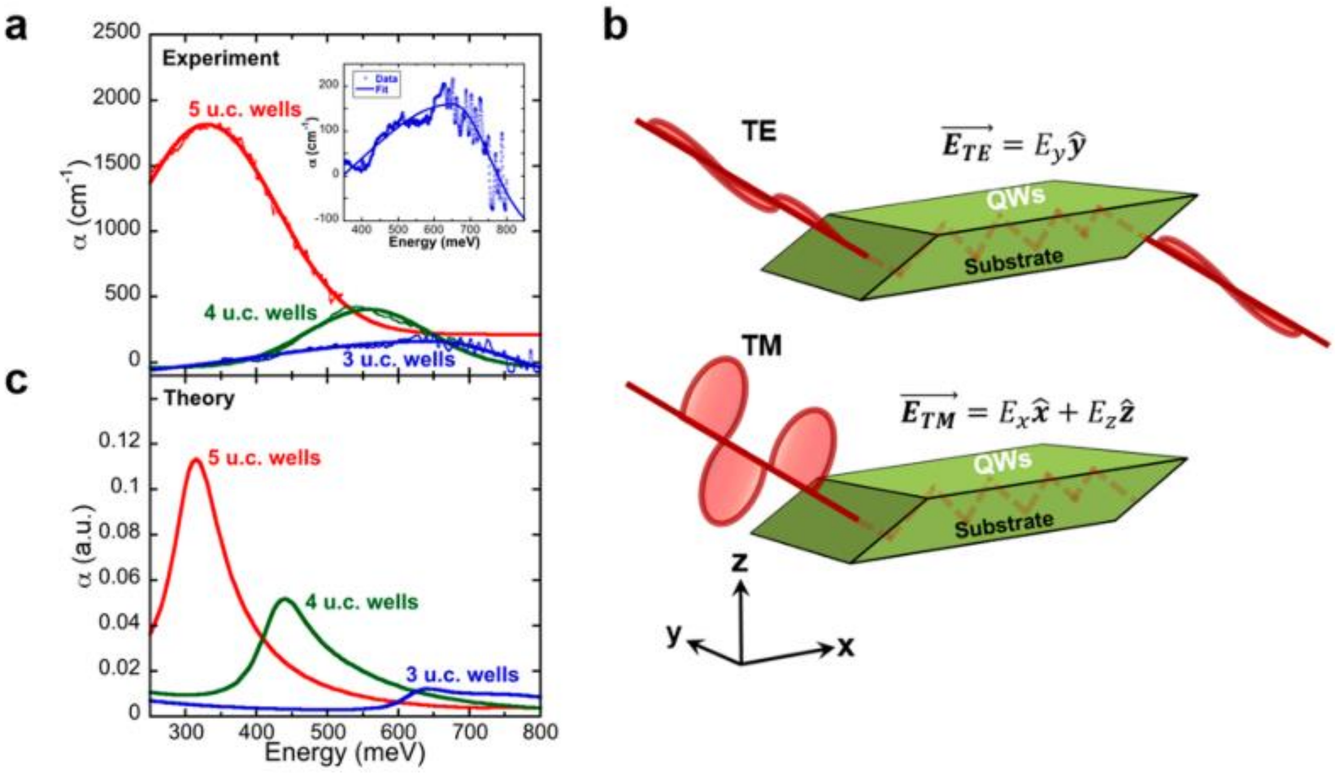
- Binary map generated from *A*-site intensities
- Bimodal distribution of well widths
- $\overline{d} = 4.32 \pm 0.63 \text{ u.c.}$
- $\sigma_n = 0.24 \pm 0.25 \text{ u.c.}$
- $\sigma_p = 0.34 \pm 0.26 \text{ u.c.}$

Recall:



Ortmann, *et al.*, *ACS Nano* **12**, 7682 (2018)
Nakagawa, *et al.*, *Nature Materials* **5**, 204 (2006)

Intersubband Absorption

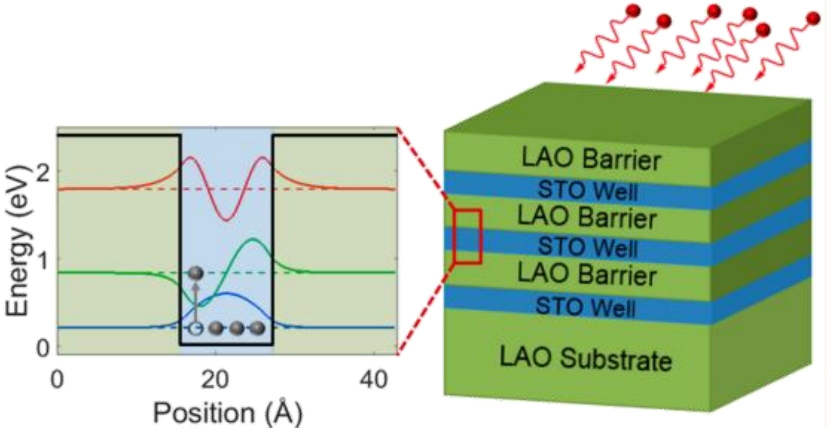


Absorption Experiments

- Spectra collected twice: once with TE and once with TM linear polarization
- Normalization suggests intersubband transitions
- Absorption energy scales appropriately

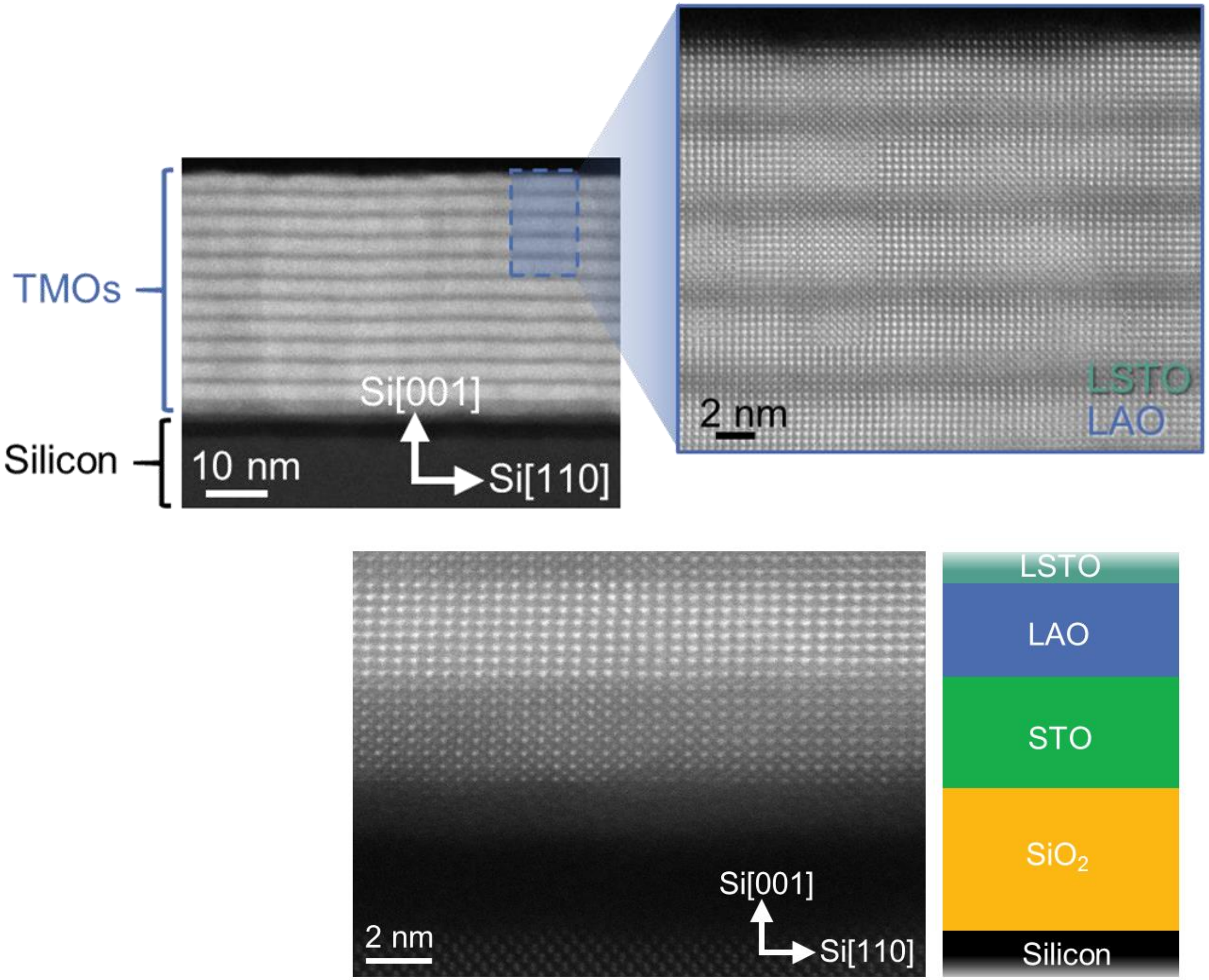
Theory

- TB calculations
- Peak position agrees well with experiment
- Peak amplitude agrees well with experiment



Ortmann, *et al.*, *ACS Nano* **12**, 7682 (2018)

Silicon-Integrated STO/LAO QWs

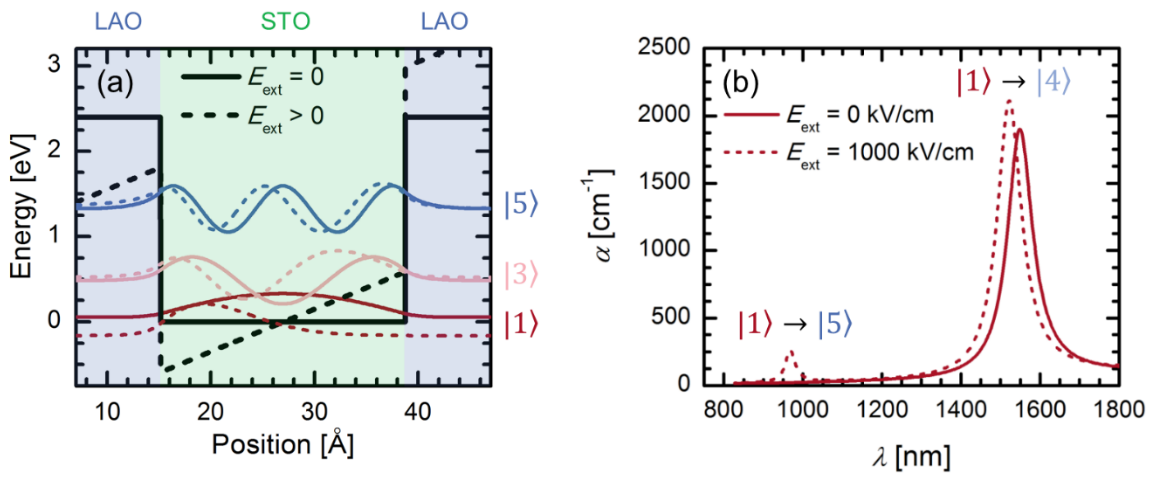


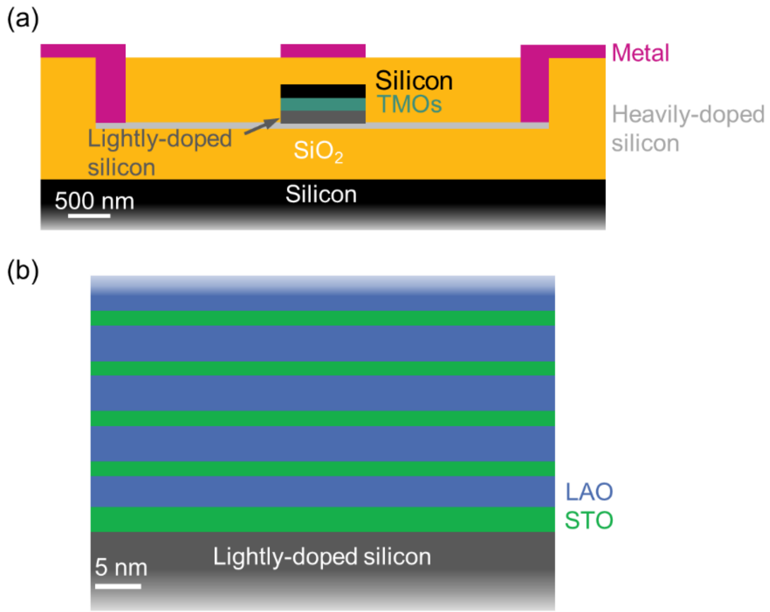
Structure

- STEM imaging shows clear STO/LAO separation
- Mosaicity observed
- SiO_2 interlayer formed
  - Can be minimized

Ortmann, *et al.*, *JAP* **125**, 155302 (2019)

Example: Integrated Modulator





Operation Principle

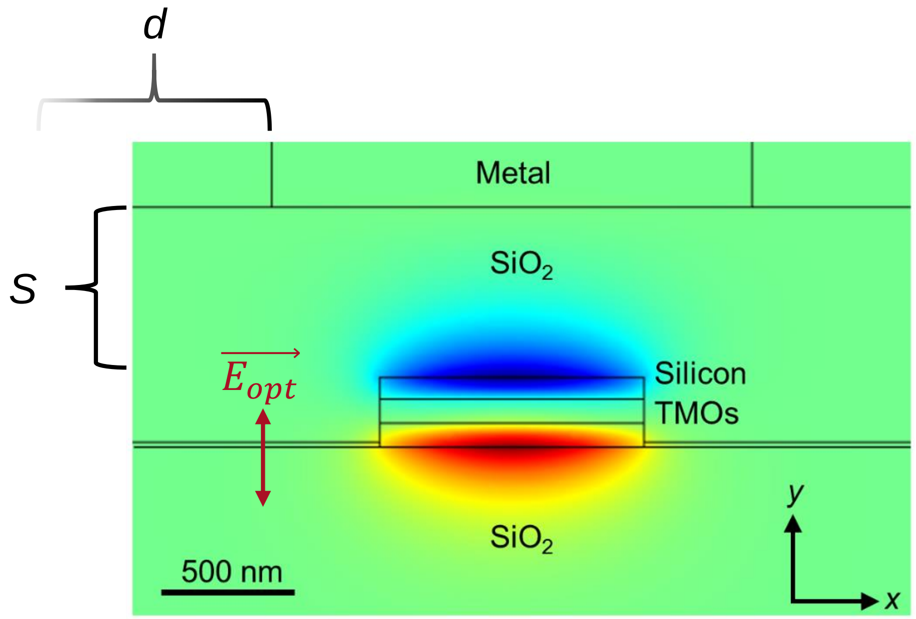
- Quantum-confined Stark effect
- Shifts intersubband transition energies
- Very fast effect

Example Device Concept

- Hybrid silicon/STO/LAO waveguide structure
- Metal electrodes

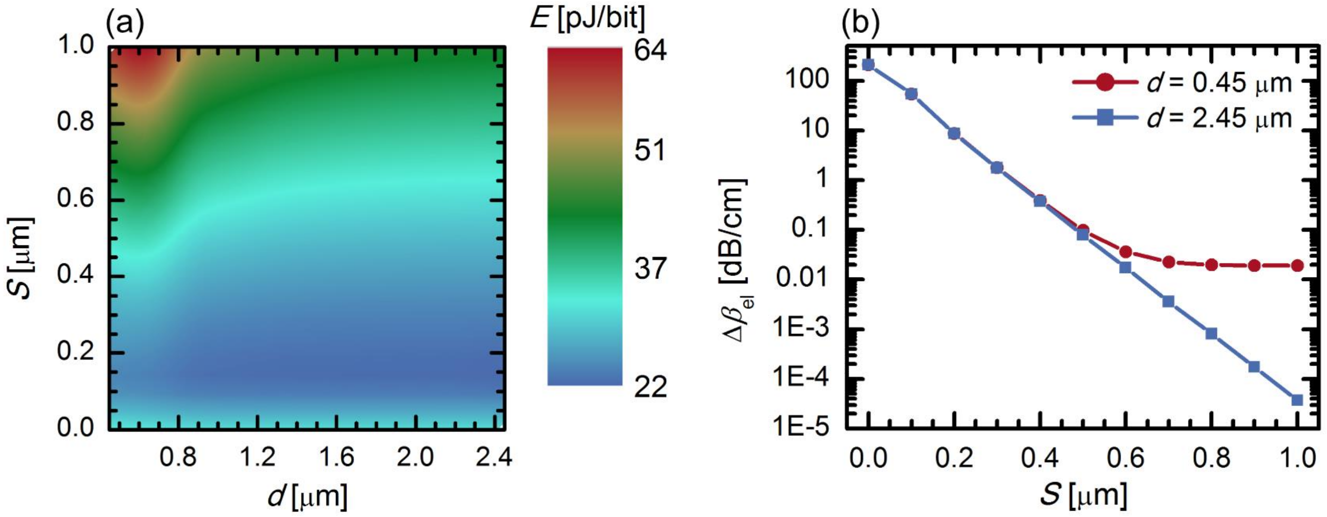
Ortmann, *et al.*, “Designing Terahertz Electro-Optic Devices from the $SrTiO_3$/$LaAlO_3$ Materials System”,Optical Materials Express **9**, 2982 (2019).

Example: Integrated Modulator

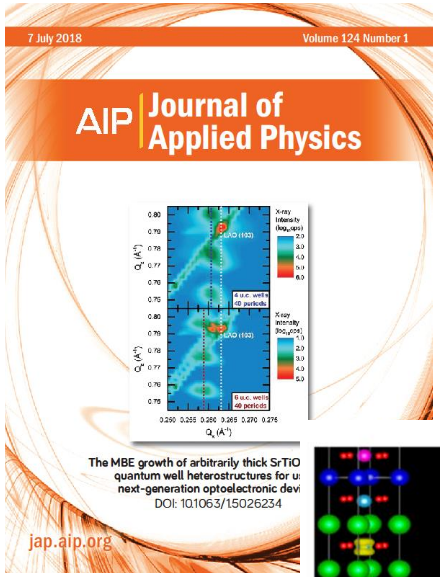


Performance Calculations

- Waveguides can support TM mode
- Energy/bit = ¼CV^2
- Energy consumption ~ 20 pJ/bit



Ortmann, *et al.*, "Designing Terahertz Electro-Optic Devices from the $SrTiO_3/LaAlO_3$ Materials System", Optical Materials Express **9**, 2982 (2019).



JOURNAL OF APPLIED PHYSICS 124, 015301 (2018)

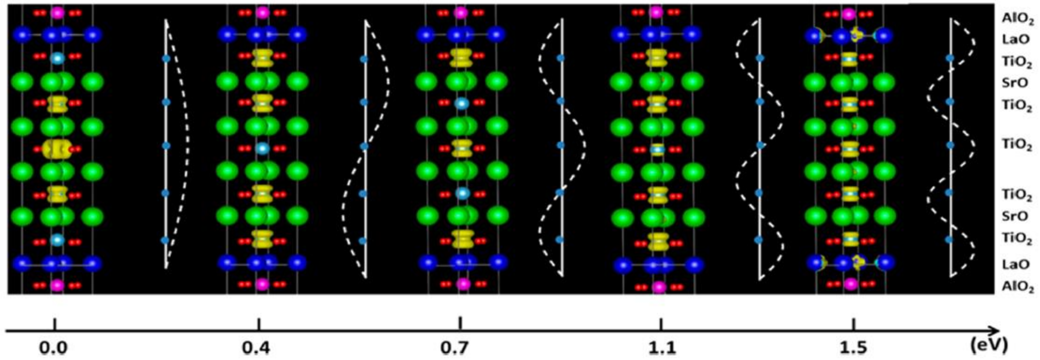
The MBE growth of arbitrarily thick $SrTiO_3/LaAlO_3$ quantum well heterostructures for use in next-generation optoelectronic devices

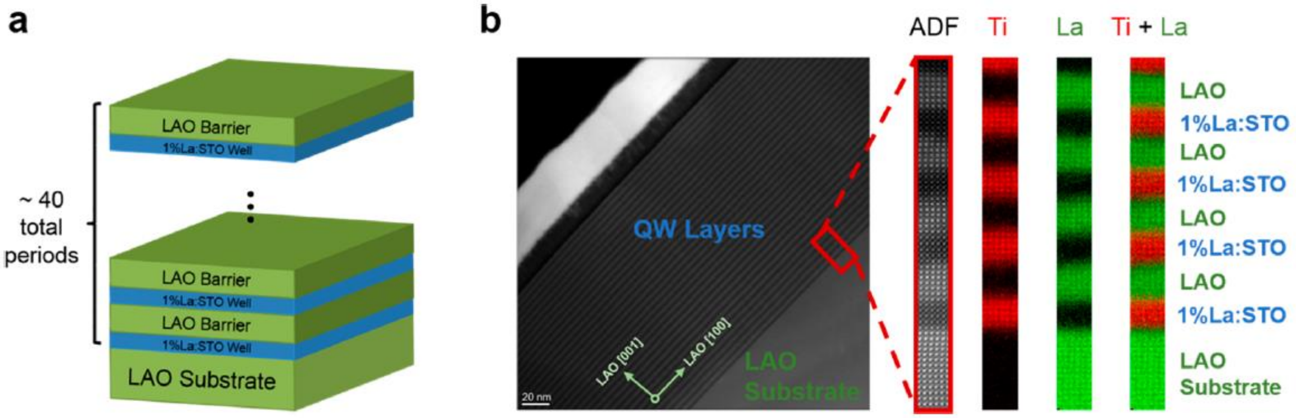
J. Elliott Ortmann, Agham B. Posadas, and Alexander A. Demkov
Department of Physics, The University of Texas, Austin, Texas 78712, USA

JOURNAL OF APPLIED PHYSICS 117, 034304 (2015)

Optical properties of transition metal oxide quantum wells

Chungwei Lin, Agham Posadas, Miri Choi, and Alexander A. Demkov
Department of Physics, University of Texas at Austin, Austin, Texas 78712, USA





APPLIED PHYSICS LETTERS 106, 192902 (2015)

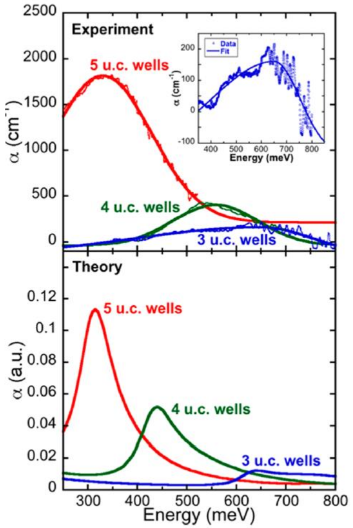
Quantum confinement in transition metal oxide quantum wells

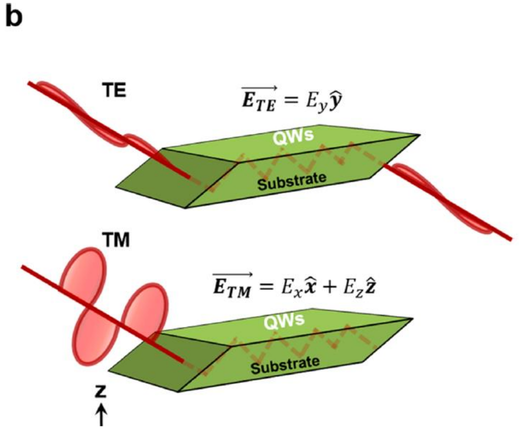
Miri Choi,[1] Chungwei Lin,[1] Matthew Butcher,[1] Cesar Rodriguez,[2] Qian He,[3] Agham B. Posadas,[1] Albina Y. Borisevich,[3] Stefan Zollner,[2] and Alexander A. Demkov[1,a)]
[1]*Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA*
[2]*Department of Physics, New Mexico State University, Las Cruces, New Mexico 88003, USA*
[3]*Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

ACS NANO
Cite This: ACS Nano 2018, 12, 7682–7689
www.acsnano.org
ARTICLE

Quantum Confinement in Oxide Heterostructures: Room-Temperature Intersubband Absorption in $SrTiO_3/LaAlO_3$ Multiple Quantum Wells

J. Elliott Ortmann,[†] Nishant Nookala,[‡,§] Qian He,[∥] Lingyuan Gao,[†] Chungwei Lin,[†,⊥] Agham B. Posadas,[†] Albina Y. Borisevich,[∥] Mikhail A. Belkin,[‡,§] and Alexander A. Demkov[*,†]





Research Article
Vol. 9, No. 7 / 1 July 2019 / Optical Materials Express 2982
Optical Materials EXPRESS

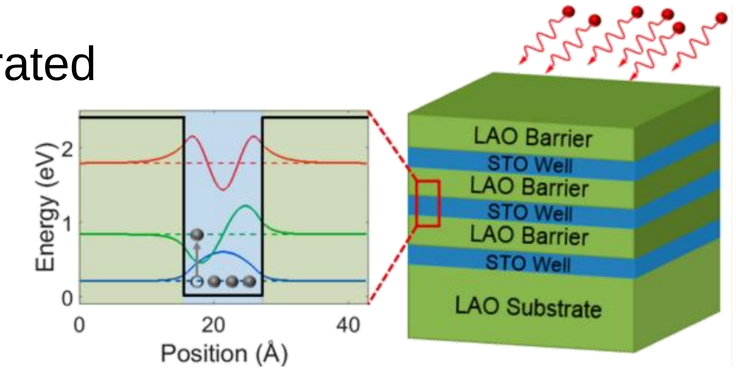
Designing near-infrared electro-optical devices from the $SrTiO_3/LaAlO_3$ materials system

J. Elliott Ortmann, Margaret A. Duncan, and Alexander A. Demkov*
Department of Physics, The University of Texas, 2515 Speedway, C1600, Austin, TX 78712, USA
*demkov@physics.utexas.edu

Summary

BTO-Based Electro-Optic Devices

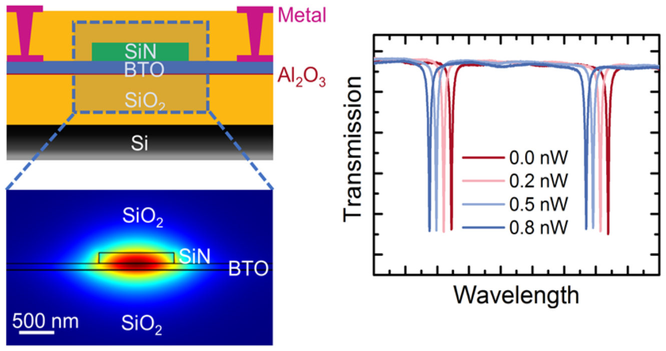
- Provided unambiguous proof that BTO retains Pockels response in integrated devices
- Measured record-high Pockels coefficient in integrated BTO devices
- Achieved ultra-low power index tuning in BTO-SiN electro-optic devices
- Measure high-speed response in BTO-SiN devices



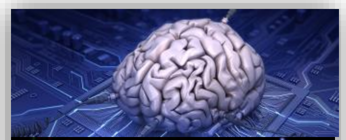
STO/LAO Quantum Wells

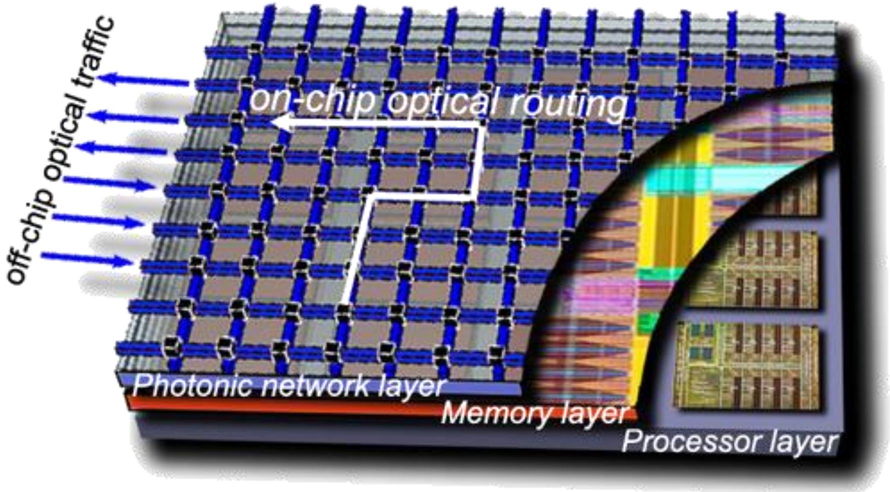
- Successfully grew high-quality, arbitrarily thick heterostructures
- Demonstrated intersubband absorption in STO/LAO QWs for first time
- Monolithically integrated STO/LAO QWs on silicon via direct deposition
- Designed and simulated STO/LAO-based integrated electro-optic devices

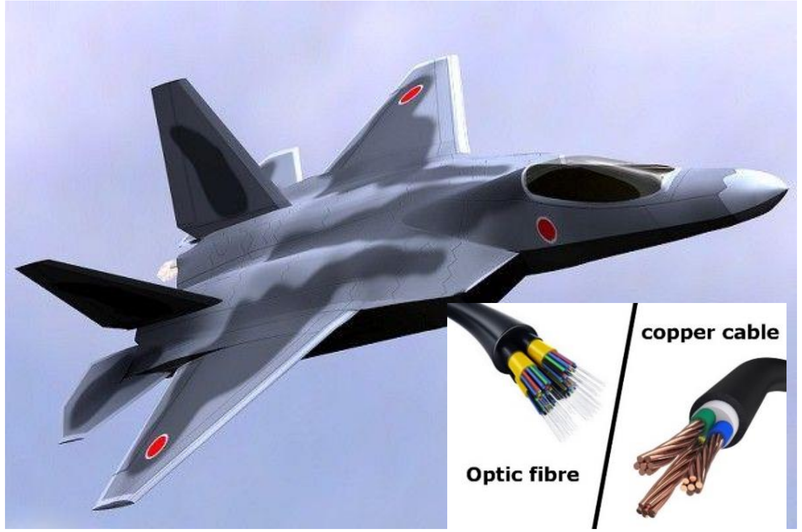
Next step: Fabricate and measure integrated devices



Thank you!




off-chip optical traffic
on-chip optical routing
Photonic network layer
Memory layer
Processor layer


copper cable
Optic fibre