From Atoms to Devices: Designing Materials for Future Devices

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Bridging scales: At the crossroads among renormalisation group, multi-scale modelling, and deep learning, 15 April 2024 — 19 April 2024

University of Colorado Boulder

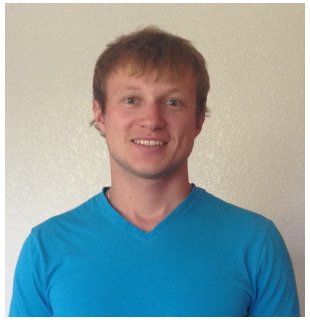
QANTAM

Thank you!



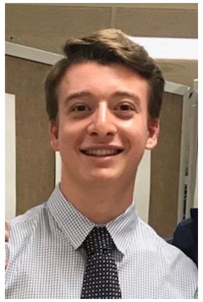
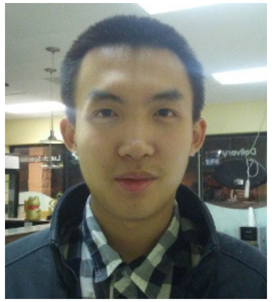



Postdoc and grad student alumni


Undergrad student alumni



Thank you!

DARPA

NSF

INTELLECTUAL VENTURES

Sandia National Laboratories

CUbit QUANTUM INITIATIVE

MFM Multi-functional Materials

XSEDE Extreme Science and Engineering Discovery Environment

U.S. Air Force Research Laboratory - DoD Supercomputing Resources

Argonne NATIONAL LABORATORY

Center for Nanoscale Materials

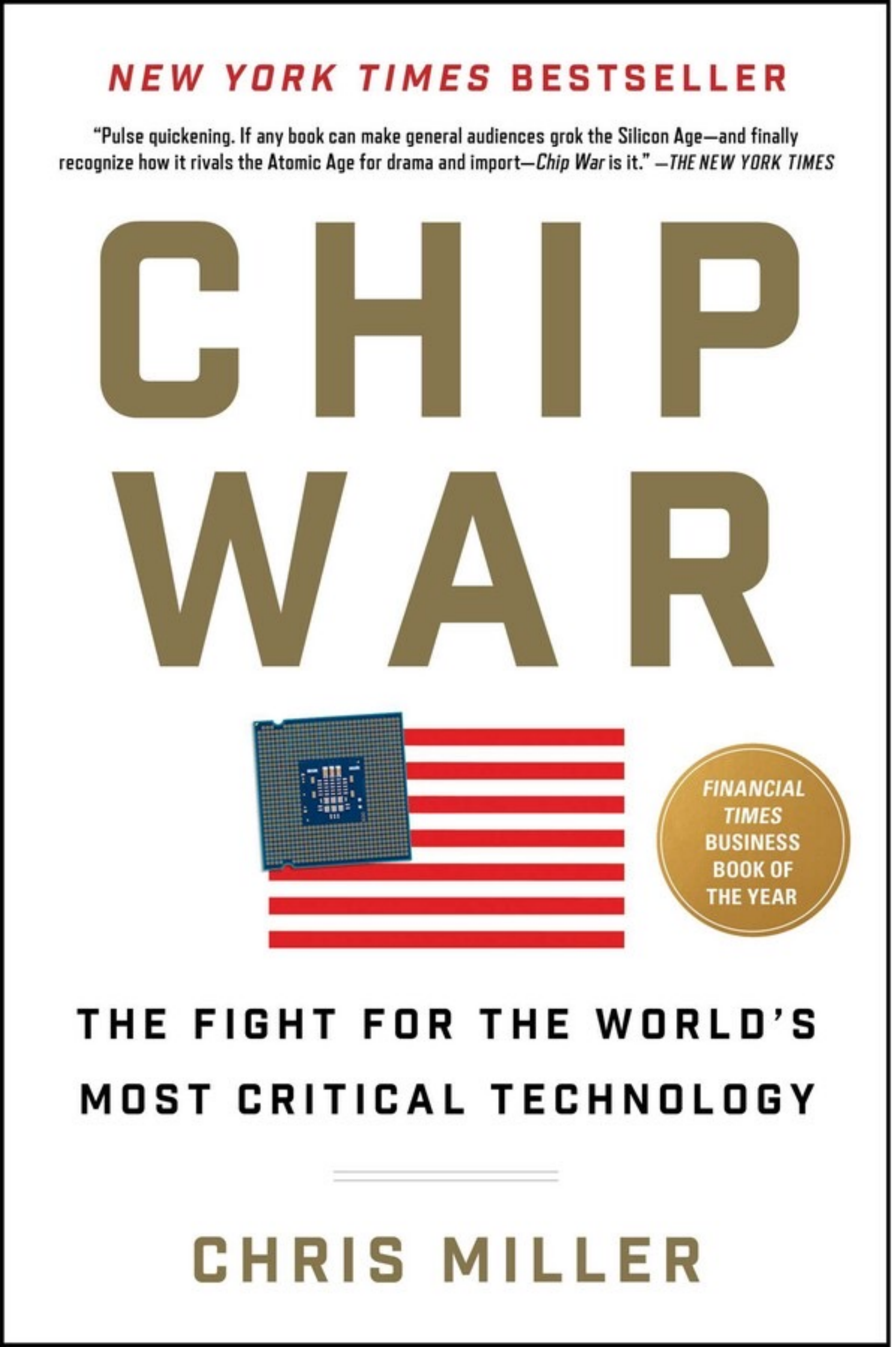
University of Colorado **Boulder**

Research Computing

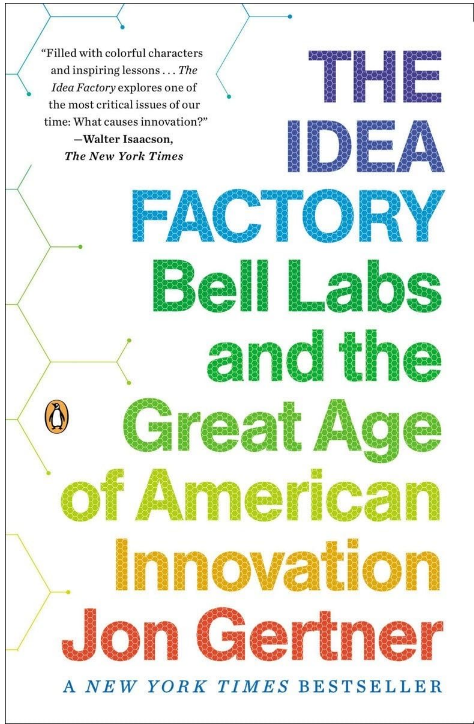
OFFICE OF INFORMATION TECHNOLOGY

From Atoms to Devices: Microchips

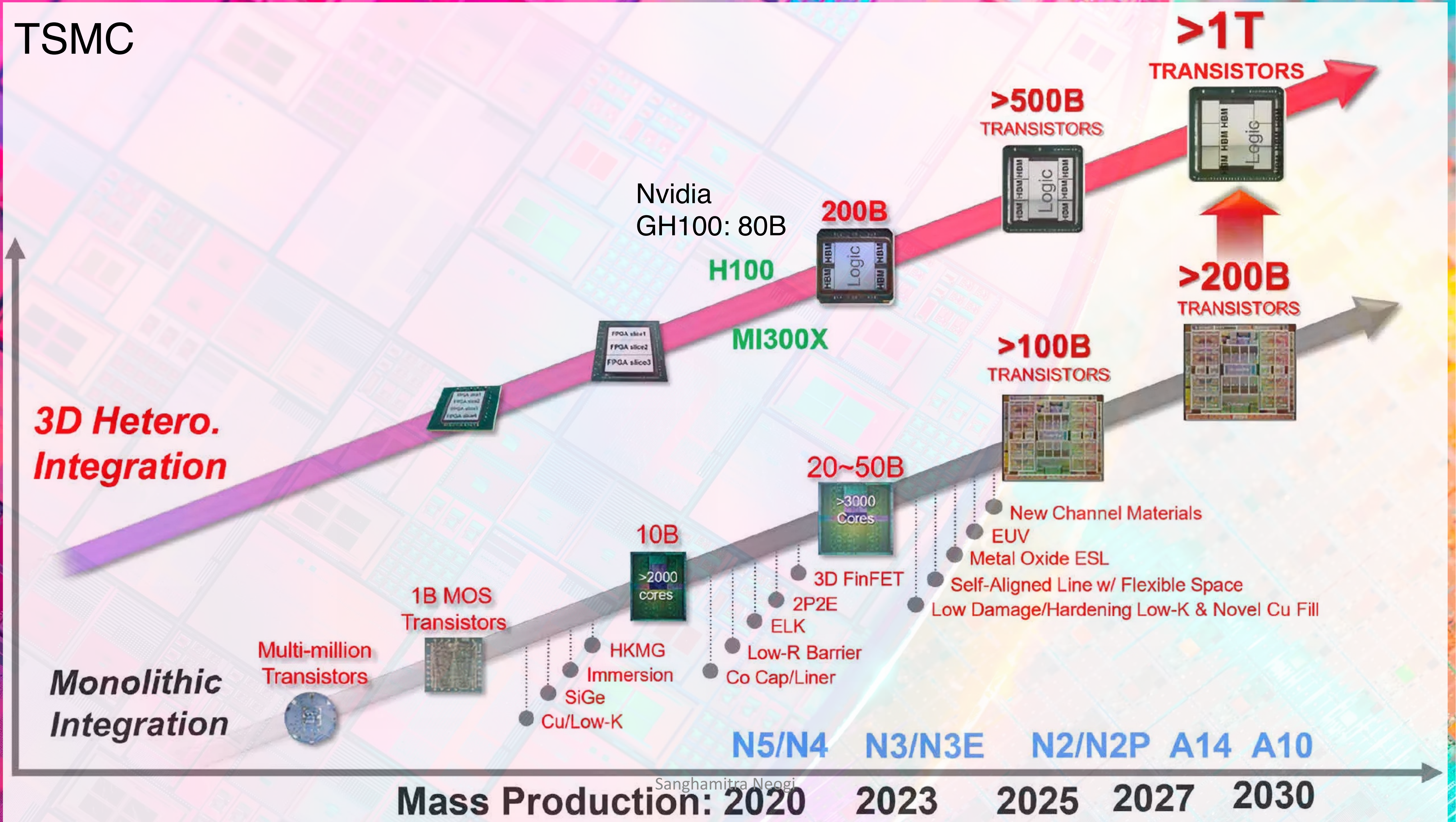
“the most complex piece of machinery ever assembled by humans.”



"Microchips are the new oil."



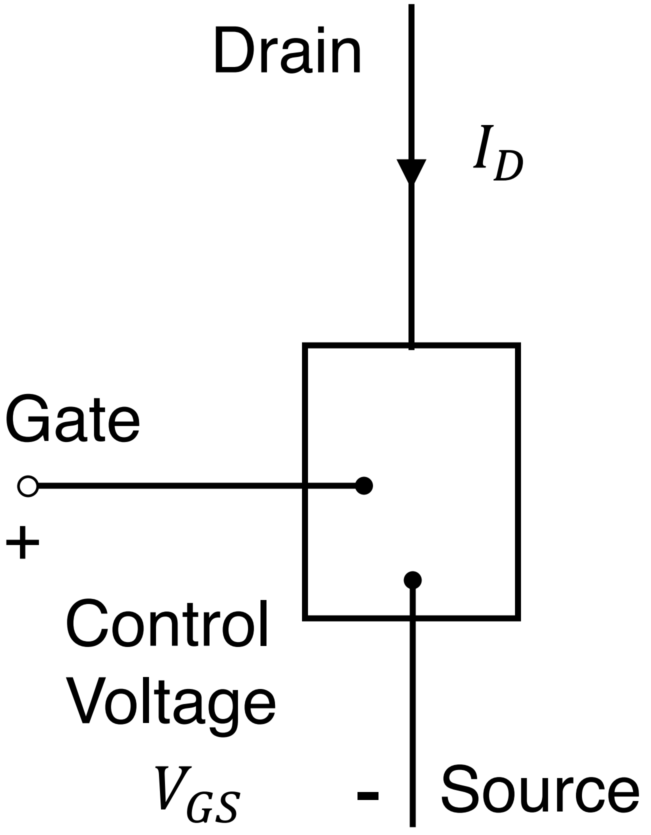
TSMC



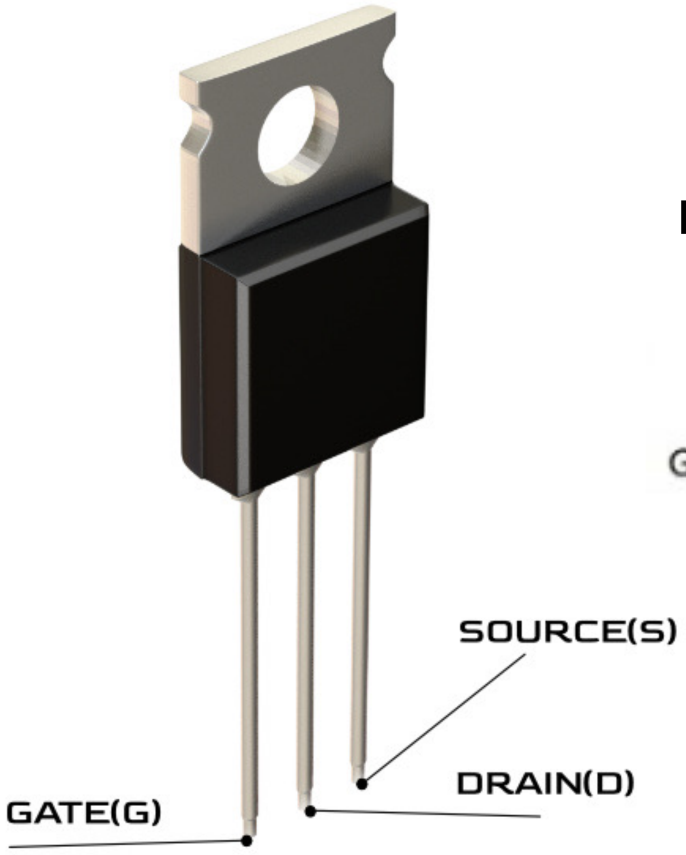
Sanghamitra Neogi

Transistors-101

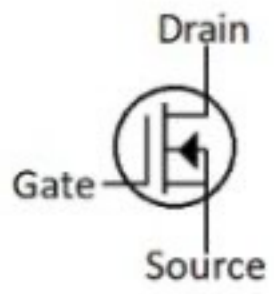
Field-Effect Transistor (FET)
Voltage-controlled amplifiers



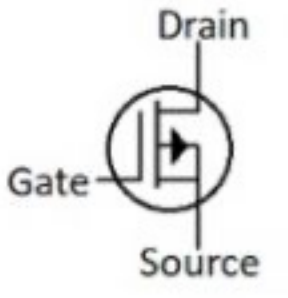
Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET)



n-channel



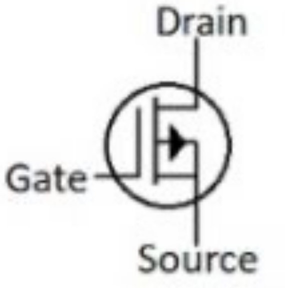
p-channel

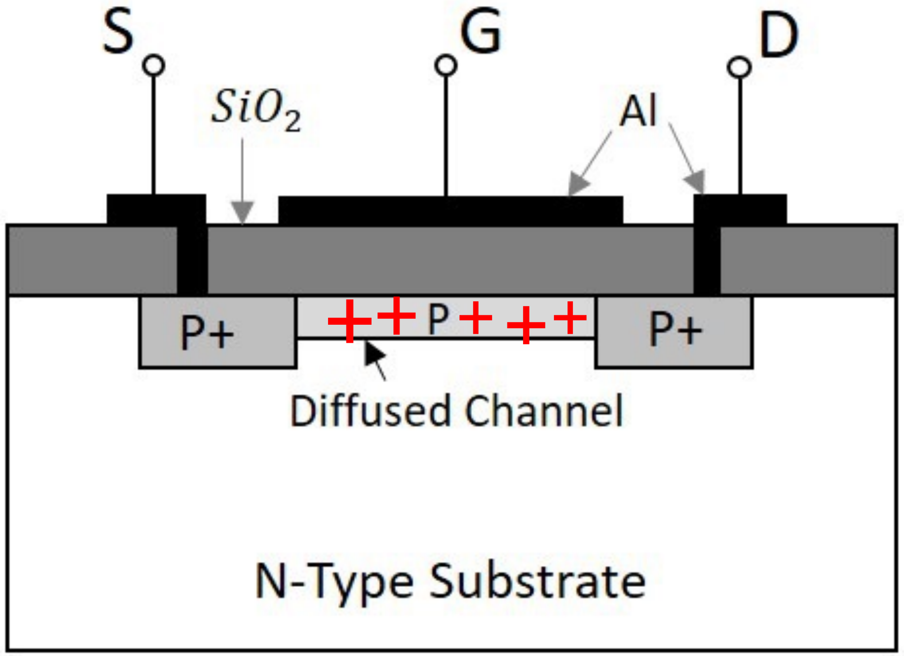


Transistors-101

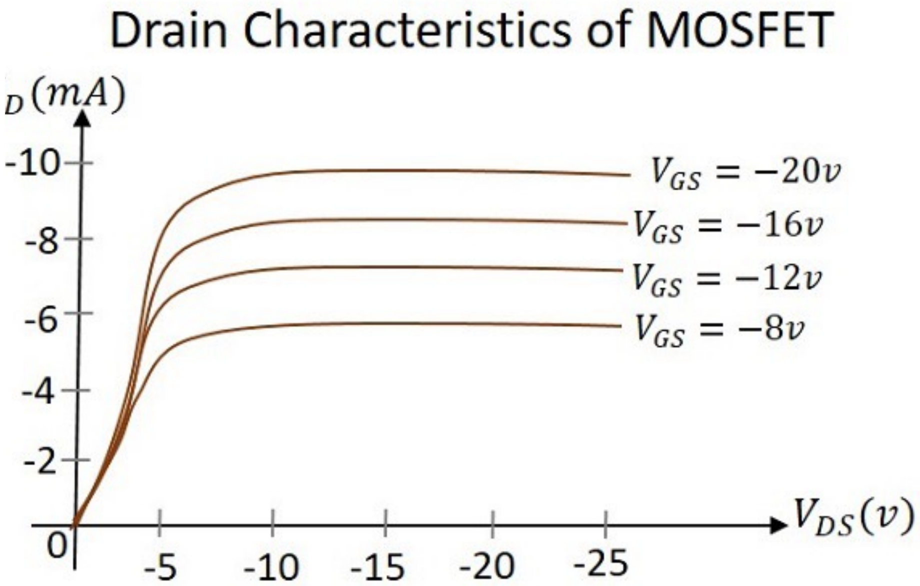
Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET)

p-channel



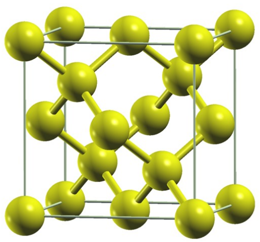


Structure of P-channel MOSFET

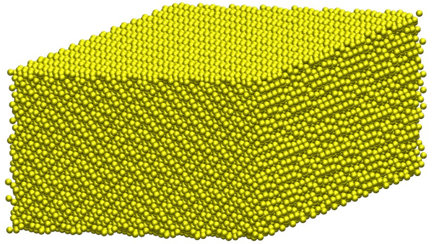


From Atoms to Devices

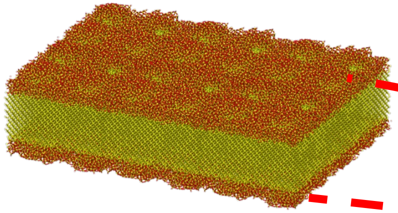
Bulk Silicon



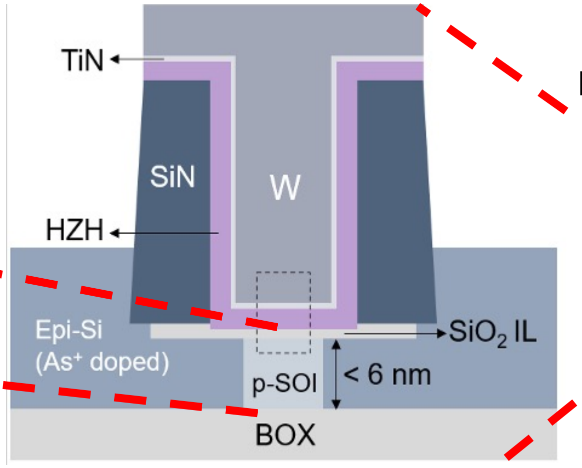
Silicon Channel



Silicon Channel Heterostructure

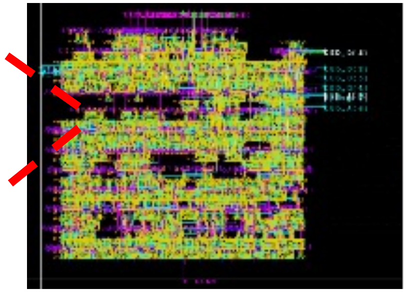


Field Effect Transistor



~size of a Coronavirus

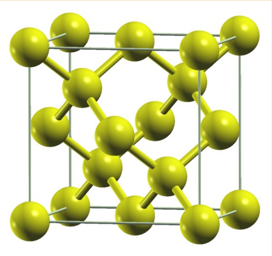
Chip/Chiplet/Circuit



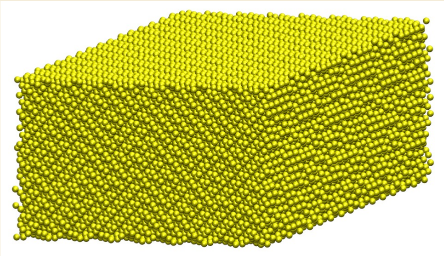
iPhone has 15 billion transistors on the main chip

From Atoms to Devices: Our Efforts

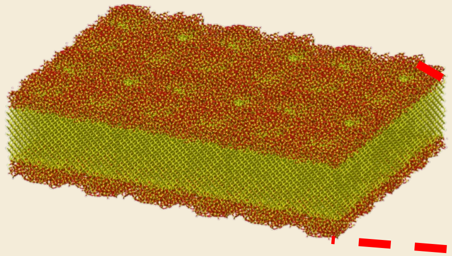
Bulk Silicon



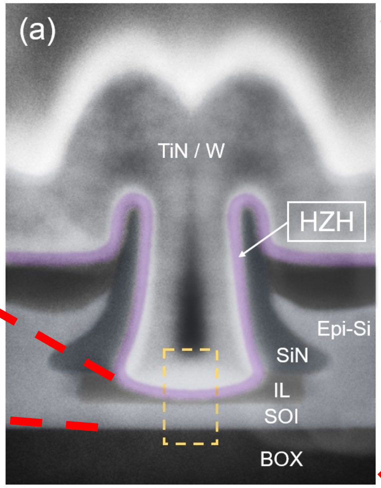
Silicon Channel



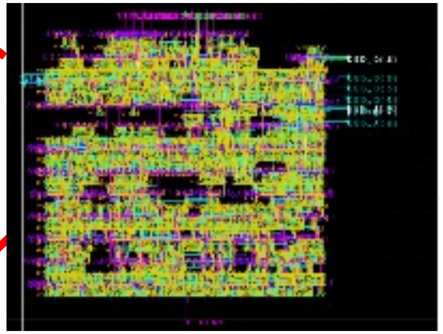
Silicon Channel Heterostructure



Field Effect Transistor



Chip/Chiplet/Circuit



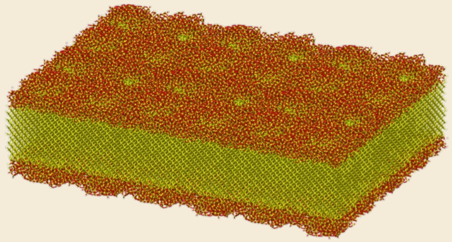
1. Atoms-to-Structures: Thermal and Electronic Properties of Semiconductor Heterostructures

ACS Nano **9** (4), 3820-3828 (2015)
EPJB **88** (3) 73 (2015)

Appl. Phys. Lett. **109**, 053902 (2016)
Phys. Rev. B, **95**(18), 180301 (2017)

Phys. Rev. B, **99**(1), 014207 (2019)
Phys. Rev. Applied **14**, 024004 (2020)

Silicon
Nanostructures



1. Thermal Properties of Semiconductor Heterostructures

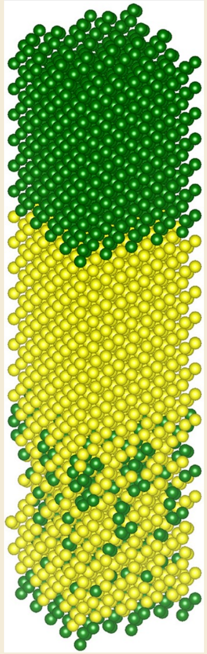
Phys. Rev. B, **99**(1), 014207 (2019)
Appl. Phys. Lett. **115**, 211602 (2019)

J. Electron Mater, **49**, 4431-4442 (2020)
J. Appl. Phys. **129**, 025301 (2021)

J. Mater. Chem. C,**10**, 7525-7542 (2022)
arXiv:2302.00261 (2023)

npj Comput. Mater. **7**, 93 (2021)

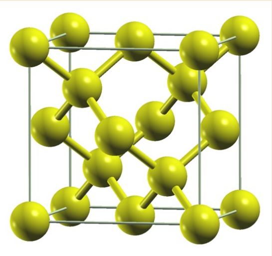
Silicon Heterostructures



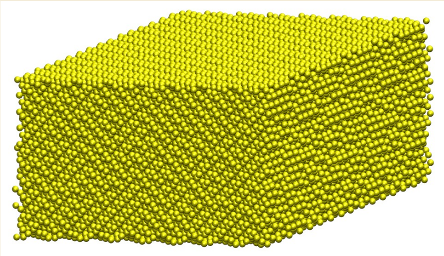
2. Electronic Properties of Semiconductor Heterostructures

From Atoms to Devices: Our Efforts

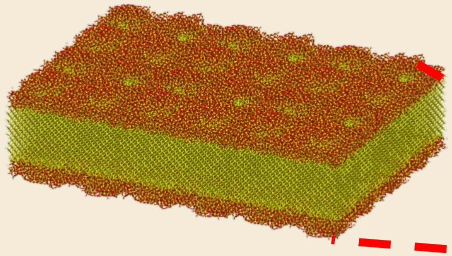
Bulk Silicon



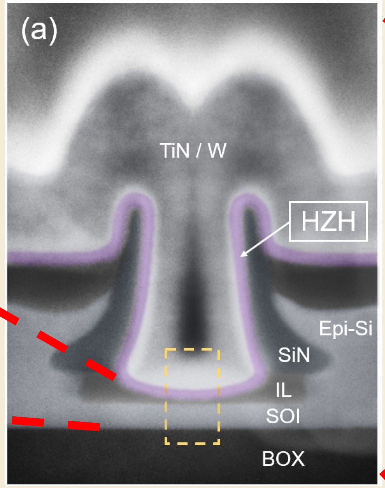
Silicon Channel



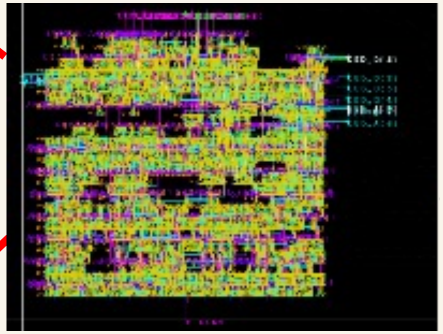
Silicon Channel with Insulating Layer



Field Effect Transistor



Chip/Chiplet/Circuit



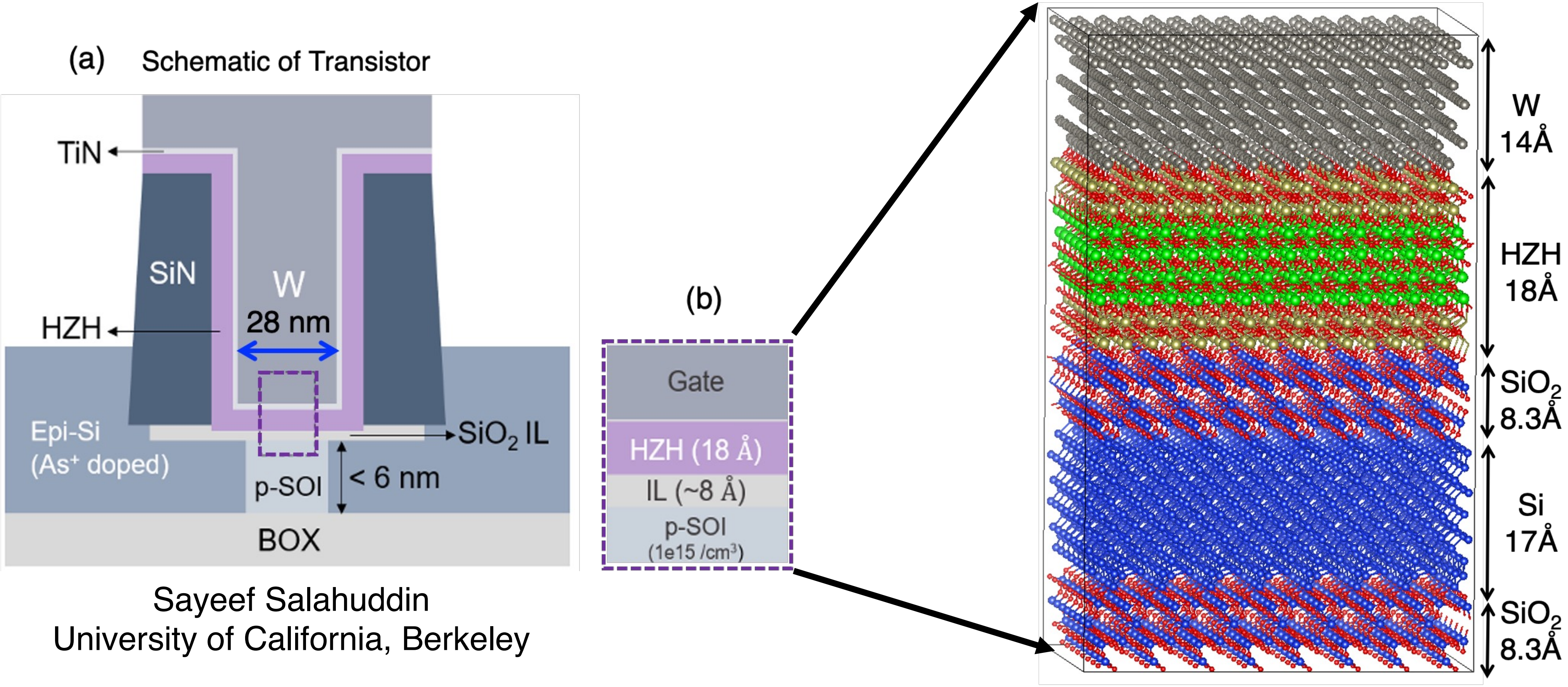
University of California, Berkeley

Purdue University

3. Atoms-to-Circuit: Thermal Model of Microelectronic Systems

DARPA

Atomistic Model of Transistor

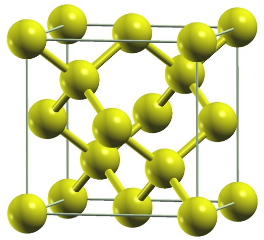


Sayeef Salahuddin
University of California, Berkeley

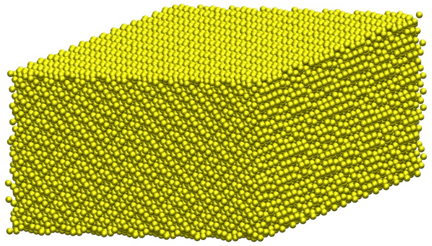
Accelerated learning of interactions using GPUs and machine learning (ML) potentials

From Atoms to Devices: Our Efforts

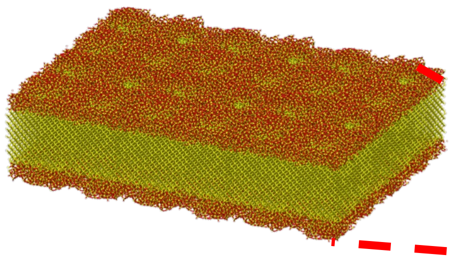
Bulk Silicon



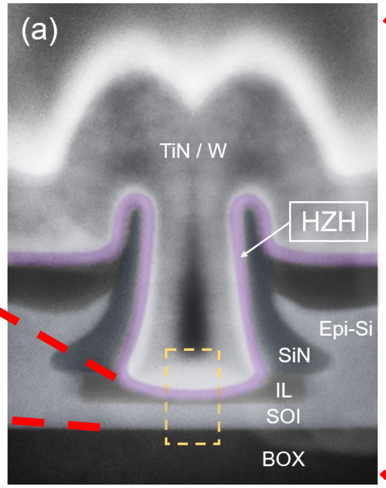
Silicon Channel



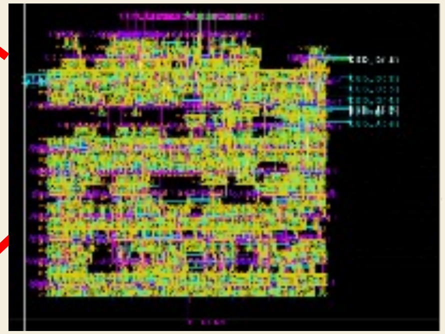
Silicon Channel with Insulating Layer



Field Effect Transistor



Chip/Chiplet/Circuit



4. Reverse model: Predicting thermal properties of structural images

Outline

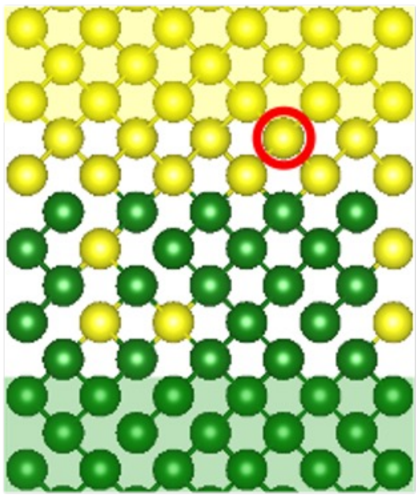
1. Atoms-to-Structures: Electronic Properties of Semiconductor Heterostructures

2. Reverse model: Predicting thermal properties of structural images

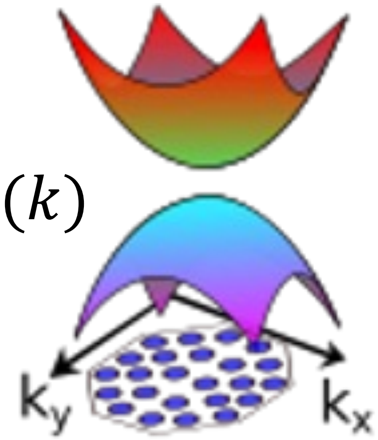
Outline

1. Atoms-to-Structures: Electronic Properties of Semiconductor Heterostructures

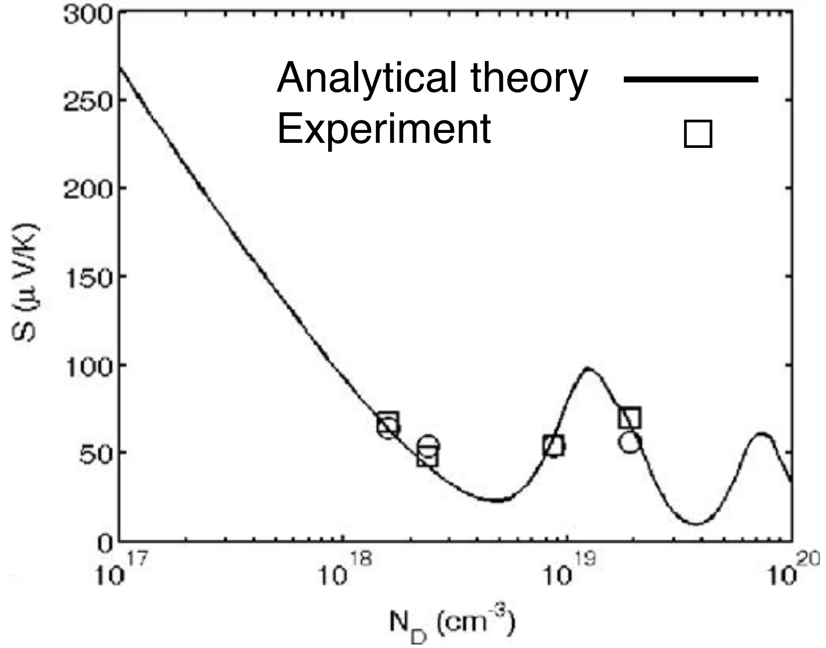
Electronic Transport Property Calculation



$E(k)$



Brillouin zone sampling



S : Seebeck coefficient or thermopower

$$S = -\frac{\Delta V}{\Delta T}$$

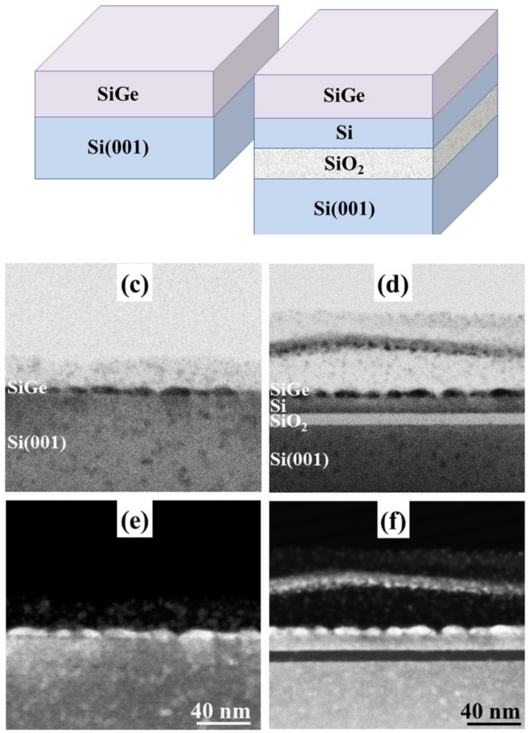
$$\propto \int_{BZ} \frac{d^3k}{4\pi^3} (E(k) - \mu)^a v(k) v(k) \tau(k) \left(-\frac{\partial f_\mu}{\partial E(k)}\right)$$

Structural Features of Heterostructures

Presence of islands

TEM

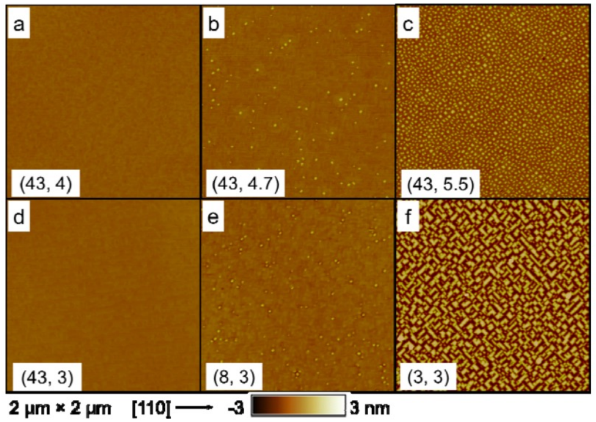
ADF



Sci Rep **8**, 2891 (2018)

Presence of nanodots

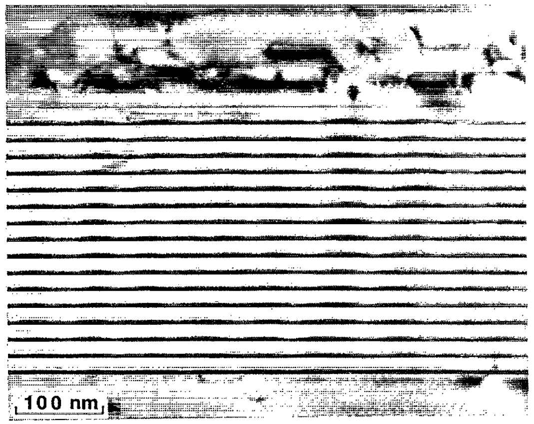
AFM



(Si)m/(Ge)n SLs
grown on Si(001)

Phys. Rev. Lett. **111**, 115901 (2013)

Rough interfaces

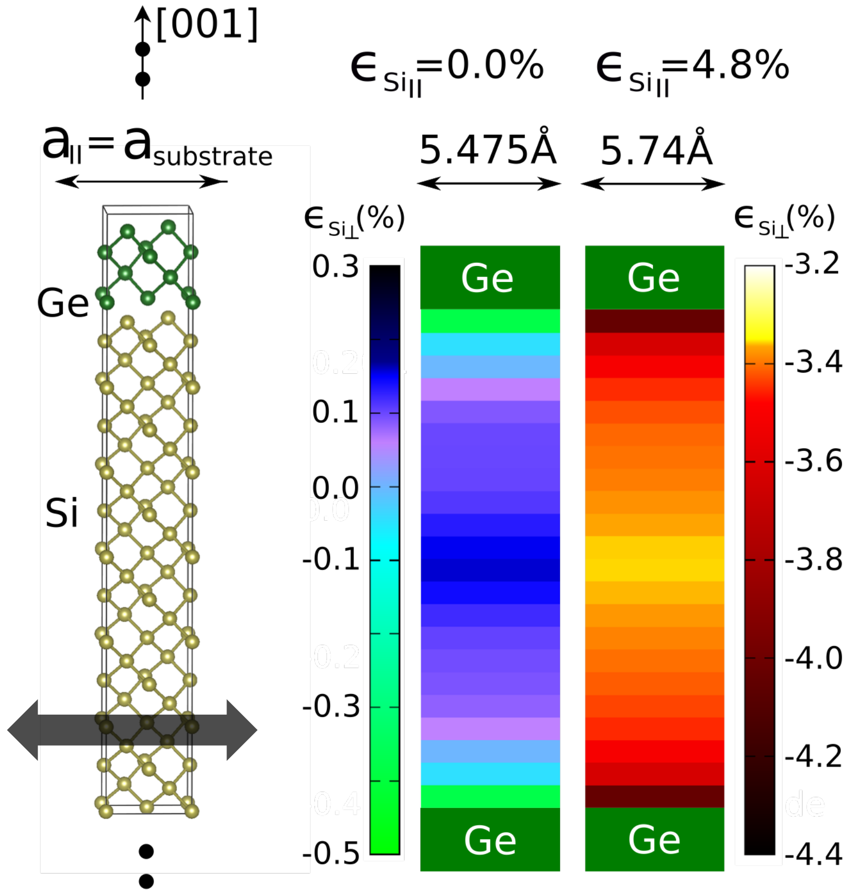


$Si_{0.5}Ge_{0.5}$(6nm)/Si (14nm)
grown on Si(001)

Appl. Phys. Lett., **59** (18), 2242 (1991)

Local Structure of Superlattices

Si_{24}/Ge_4
superlattice



Strain in Si region

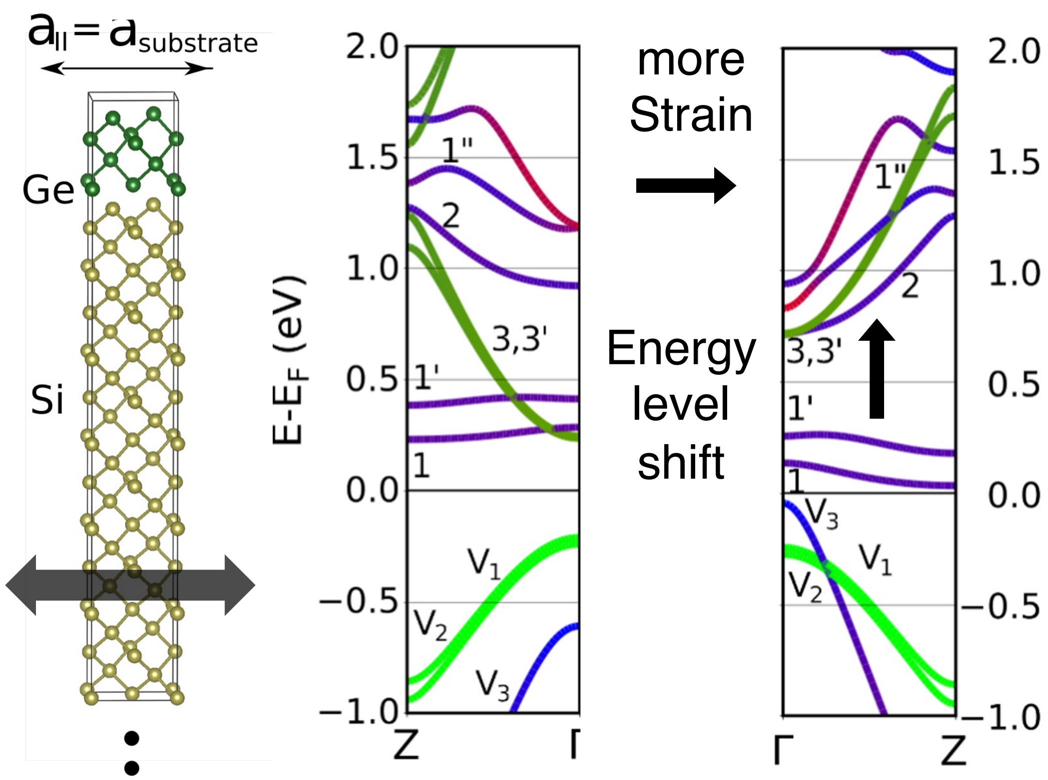
on Si (001) on Ge (001)

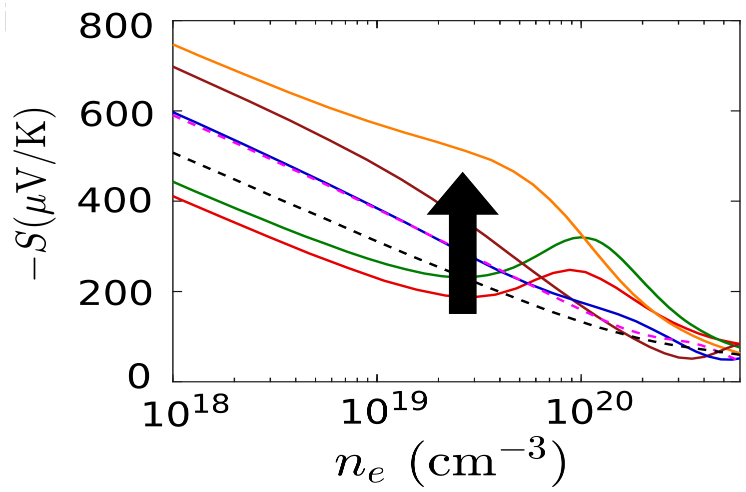
non-uniform
local strain in
heterostructure

Structure-Electronic Property Relationships

QUANTUMESPRESSO

BoltzTrap



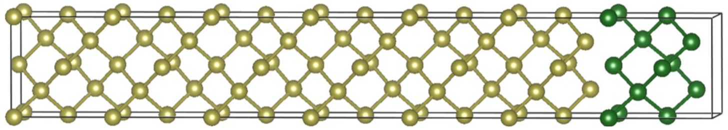


Modulated Seebeck Coefficient

Electronic transport of semiconductor heterostructures can be tuned using strain

Approach

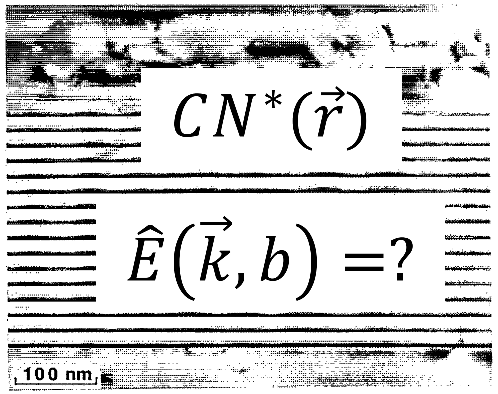
Model systems



Local environment: $CN(\vec{r})$

Energy bands: $E(\vec{k}, b)$

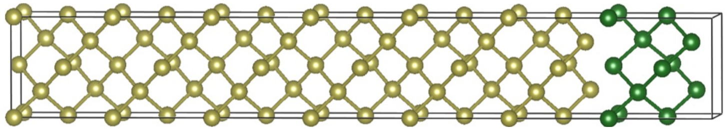
Experimental heterostructures



Hypothesis: Local structure-energy bands relationships, $f(CN(\vec{r}), E)$, are transferable

Approach

Model systems



Local environment: $CN(\vec{r})$

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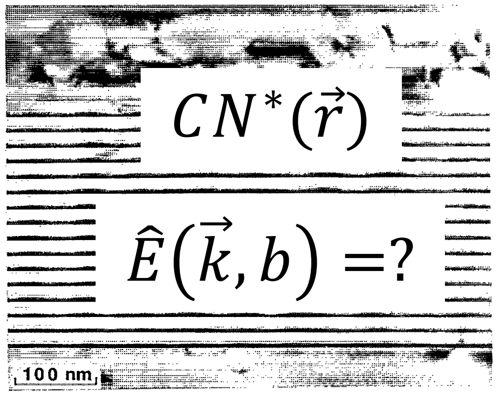
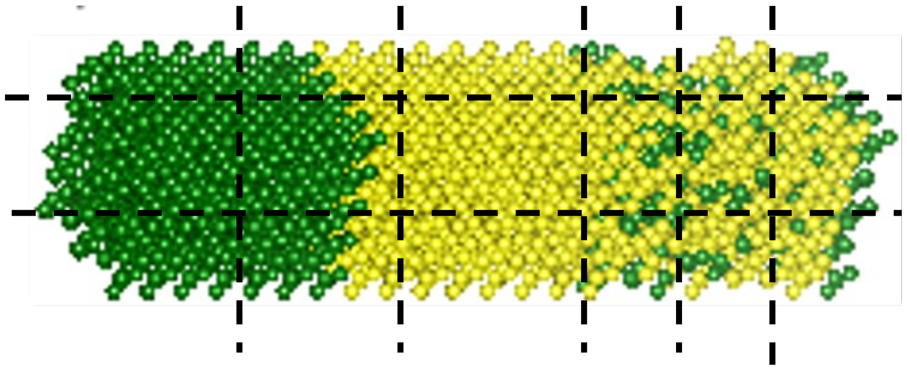
Experimental heterostructures



1. Train ML models to predict $f(CN(\vec{r}), E)$, for unknown local environments
2. Sum local properties to get global properties

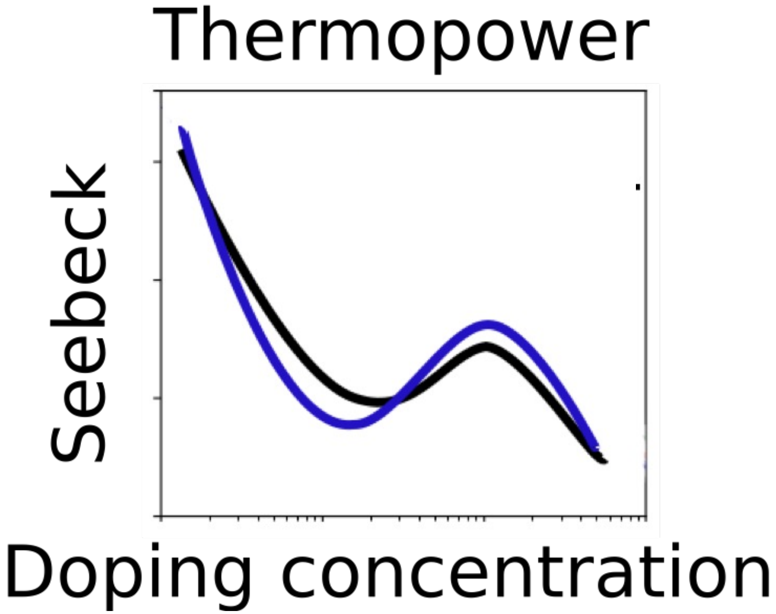
Forward Electronic Transport ML Model



~600 atoms

16-atom Si/Ge ordered and disordered units

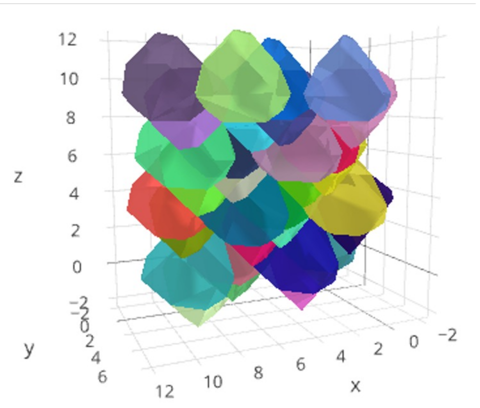
ML model



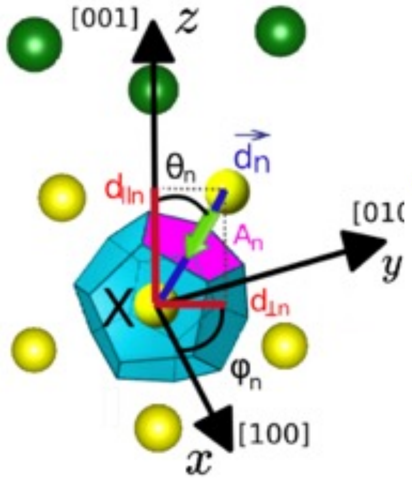
ML model extrapolates structure-electronic property relationships to larger systems, bypassing expensive computation

Descriptors of $\mathrm{CN}(\vec{r})$

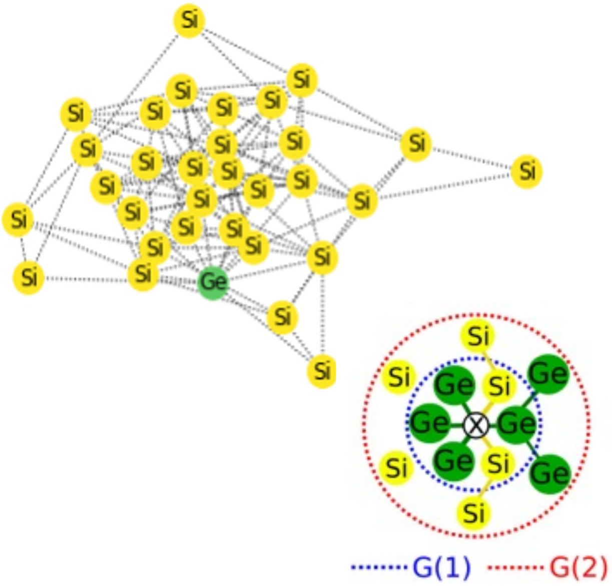
Voronoi tessellation (VT)



Voronoi cell



Crystal graph



1. Perform VT of crystal structure
2. Calculate statistics of VT derived attributes
3. Construct CG through adjacent cells
4. Calculate order parameters

Phys. Rev. **77**, 669 (1950)

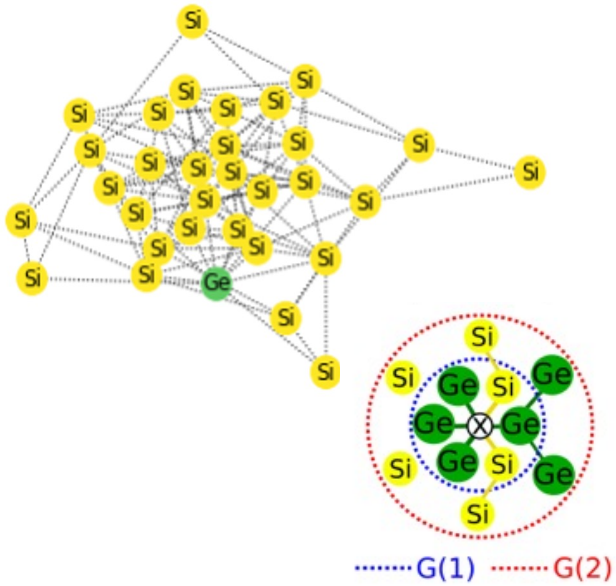
Phys. Rev. B **96**, 024104 (2017)

npj Comput Mater **7**, 93 (2021)

https://github.com/CUANTAM/Crystal-Graph-Features

Adequate Representations: Directionality

Crystal graph



Order parameters

$$Q_X^{\Omega,\mathrm{order}} = \sum_{\substack{\mathrm{paths} \\ \mathrm{in\ CG}}} \prod_{\mathrm{steps}}^{\mathrm{order}} \frac{\overrightarrow{\omega_n} A_n \overbrace{\delta_{n,X}}^{\text{species aware}}}{\underbrace{\sum_{\mathrm{Cell}} \overrightarrow{\omega_a} A_a}_{\text{all steps}} - \underbrace{\sum_{\mathrm{cell}} \overrightarrow{\omega_b} A_b}_{\text{backtracking steps}}}$$

Directional bias:

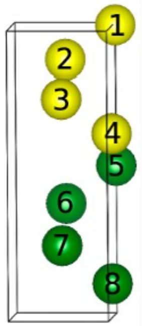
$$\overrightarrow{\omega_n} = (|\cos\phi_n \sin\theta_n|, |\sin\phi_n \sin\theta_n|, |\cos\theta_n|)$$

- Unique representation of $\mathrm{CN}(\vec{r})$
- Quantify proximity to an interface
- Representative of directionality or inhomogeneity
- Scalable to large system sizes
- Obtainable from imaging data

npj Comput Mater **7**, 93 (2021)

https://github.com/CUANTAM/Crystal-Graph-Features

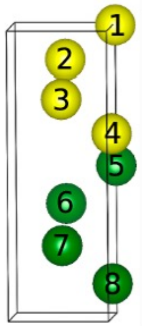
Descriptors of $\mathrm{CN}(\vec{r})$: Input to ML



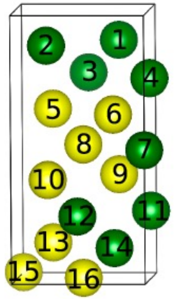
Atom	#	$Q^{x,1}$	$Q^{y,1}$	$Q^{z,1}$	$Q^{x,2}$	$Q^{y,2}$	$Q^{z,2}$	$Q^{x,3}$	$Q^{y,3}$	$Q^{z,3}$
Si	1	0.55	0.55	0.51	0.49	0.49	0.45	0.36	0.36	0.29
Si	2	0.95	0.95	0.89	0.64	0.64	0.53	0.43	0.43	0.34
Si	3	0.95	0.95	0.89	0.64	0.64	0.53	0.43	0.43	0.34
Si	4	0.55	0.55	0.51	0.49	0.49	0.45	0.36	0.36	0.29
Ge	5	0.53	0.53	0.49	0.47	0.47	0.46	0.37	0.37	0.30
Ge	6	0.97	0.97	0.94	0.70	0.70	0.58	0.47	0.47	0.36
Ge	7	0.97	0.97	0.94	0.70	0.70	0.58	0.47	0.47	0.36
Ge	8	0.53	0.53	0.49	0.47	0.47	0.46	0.37	0.37	0.30

Pimachev and Neogi, *npj Comput Mater* 7, 93 (2021)
https://github.com/CUANTAM/Crystal-Graph-Features

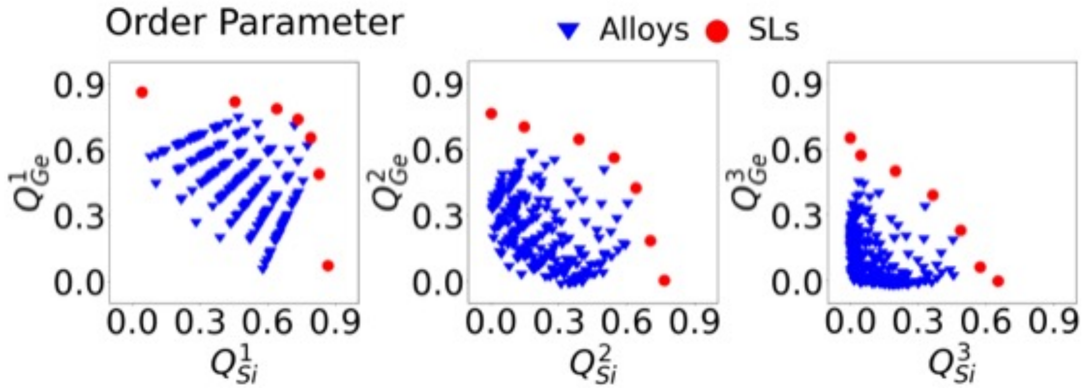
Descriptors of $\mathrm{CN}(\vec{r})$: Input to ML



Atom	#	$Q^{x,1}$	$Q^{y,1}$	$Q^{z,1}$	$Q^{x,2}$	$Q^{y,2}$	$Q^{z,2}$	$Q^{x,3}$	$Q^{y,3}$	$Q^{z,3}$
Si	1	0.55	0.55	0.51	0.49	0.49	0.45	0.36	0.36	0.29
Si	2	0.95	0.95	0.89	0.64	0.64	0.53	0.43	0.43	0.34
Si	3	0.95	0.95	0.89	0.64	0.64	0.53	0.43	0.43	0.34
Si	4	0.55	0.55	0.51	0.49	0.49	0.45	0.36	0.36	0.29
Ge	5	0.53	0.53	0.49	0.47	0.47	0.46	0.37	0.37	0.30
Ge	6	0.97	0.97	0.94	0.70	0.70	0.58	0.47	0.47	0.36
Ge	7	0.97	0.97	0.94	0.70	0.70	0.58	0.47	0.47	0.36
Ge	8	0.53	0.53	0.49	0.47	0.47	0.46	0.37	0.37	0.30



Atom	#	$Q^{x,1}$	$Q^{y,1}$	$Q^{z,1}$	$Q^{x,2}$	$Q^{y,2}$	$Q^{z,2}$	$Q^{x,3}$	$Q^{y,3}$	$Q^{z,3}$
Ge	1	0.50	0.55	0.48	0.21	0.21	0.15	0.09	0.08	0.05
Ge	2	0.55	0.50	0.48	0.23	0.21	0.17	0.08	0.08	0.04
Ge	3	0.55	0.50	0.48	0.21	0.21	0.15	0.08	0.09	0.05
Ge	4	0.50	0.55	0.48	0.21	0.23	0.17	0.08	0.08	0.04
Si	5	0.34	0.34	0.30	0.22	0.22	0.20	0.05	0.05	0.04
Si	6	0.34	0.34	0.30	0.21	0.21	0.20	0.05	0.05	0.04
Ge	7	0.10	0.10	0.19	0.05	0.05	0.08	0.02	0.02	0.03
Si	8	0.83	0.83	0.83	0.11	0.11	0.09	0.03	0.03	0.03
Si	9	0.34	0.37	0.34	0.22	0.23	0.22	0.05	0.05	0.03
Si	10	0.37	0.34	0.34	0.23	0.22	0.22	0.05	0.05	0.03
Ge	11	0.34	0.29	0.26	0.09	0.10	0.08	0.02	0.02	0.02
Ge	12	0.29	0.34	0.26	0.10	0.09	0.08	0.02	0.02	0.02
Si	13	0.45	0.45	0.49	0.05	0.05	0.03	0.02	0.02	0.02
Ge	14	0.46	0.46	0.51	0.08	0.08	0.08	0.03	0.03	0.02
Si	15	0.30	0.30	0.21	0.09	0.09	0.07	0.01	0.01	0.01
Si	16	0.30	0.30	0.21	0.09	0.09	0.07	0.01	0.01	0.01



Training ML Model

1. Global features
2. Statistical parameters of VT derived attributes
3. Statistical parameters of order parameters

$CN(\vec{r})$

4. Electronic band structures: $E(\vec{k}, b)$

Train ML models to learn $f(CN(\vec{r}), E(\vec{k}, b))$ and predict $\hat{E}(\vec{k}, b)$, given $CN^*(\vec{r})$

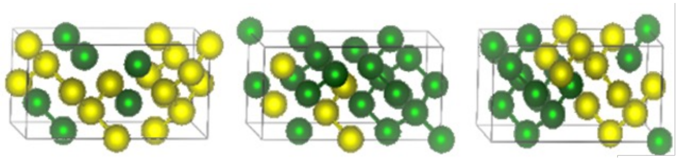
PBE exchange-correlation functional

Generalized gradient approximation

BoltzTrap

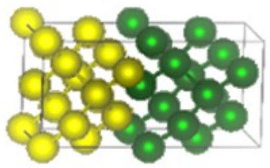
Testing Validity of Hypothesis: Transferable $f(CN(\vec{r}), E(\vec{k}, b))$ Relationships

Training set:
Si/Ge units



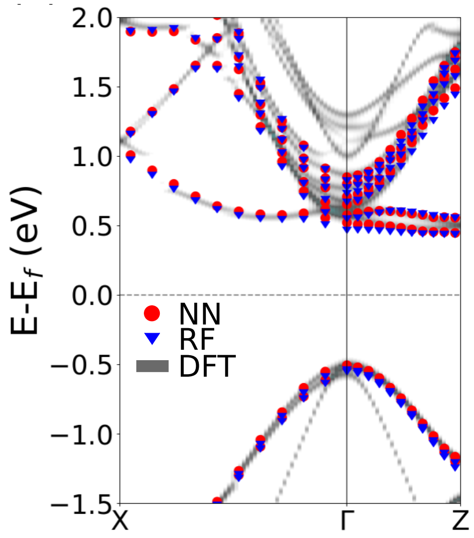
350 16-atom Si/Ge units

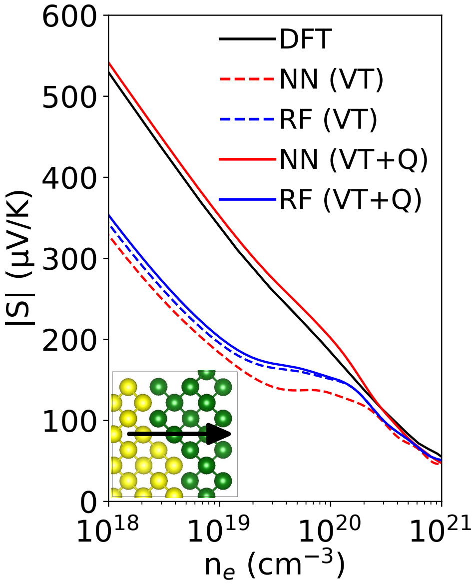
Testing structures:
Si/Ge superlattices



32-atom Si/Ge superlattice

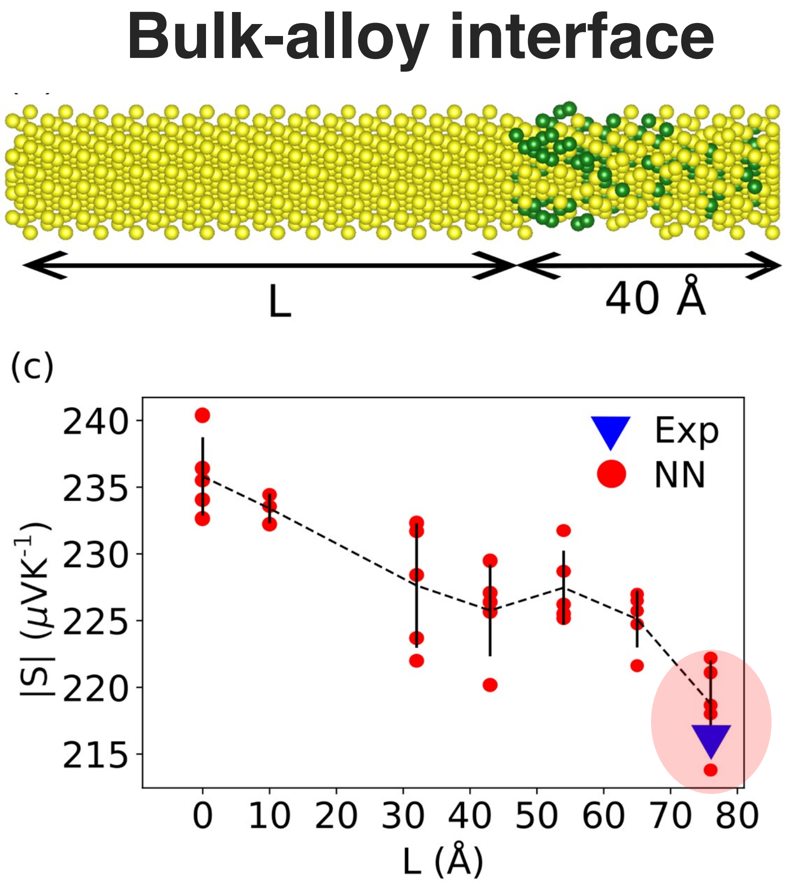
Superlattice with imperfect layers





Able to predict electronic properties of larger structures after being trained on 16-atom units

Forward Electronic Transport ML Model



ML-predicted $E(\boldsymbol{k}, \boldsymbol{b})$ used to predict electronic properties of ~600 atom semiconductor heterostructure

npj Comput. Mater. **7**, 93 (2021)

IEEE Spectrum | Physicists Teach AI to Simulate Atomic Clusters

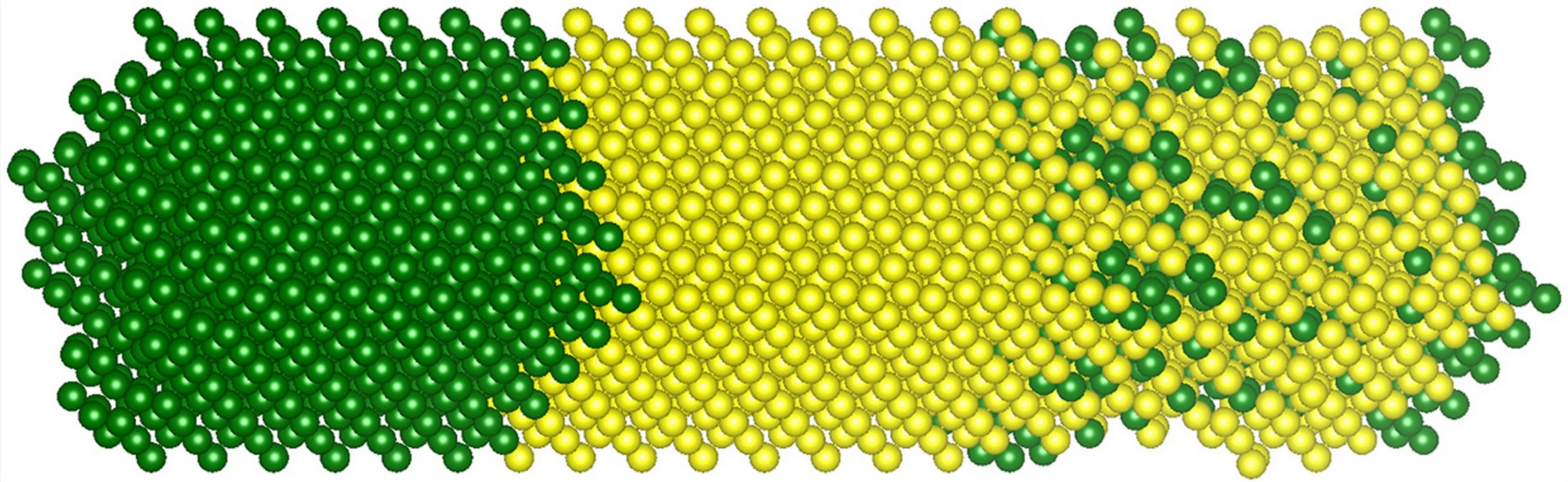
Type to search

NEWS | ARTIFICIAL INTELLIGENCE

Physicists Teach AI to Simulate Atomic Clusters ›

Physics-informed machine learning might help verify microchips

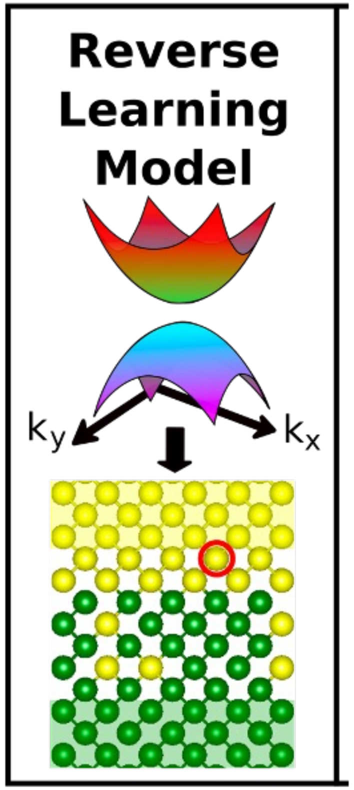
BY MATTHEW HUTSON | 02 JUL 2021 | 3 MIN READ



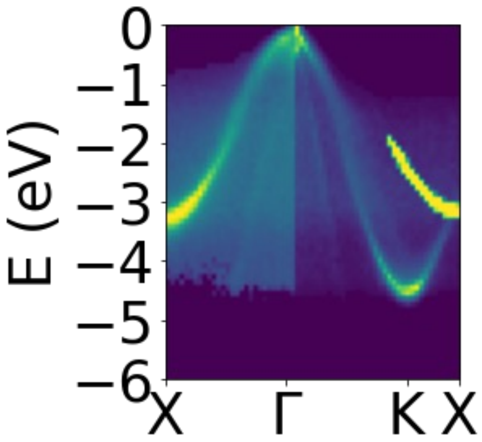
Representative configuration of a fabricated heterostructure. Target S of fabricated heterostructures are computed from $E\ (k,b)$ using BTE. UNIVERSITY OF COLORADO BOULDER/NPJ COMPUTATIONAL MATERIALS

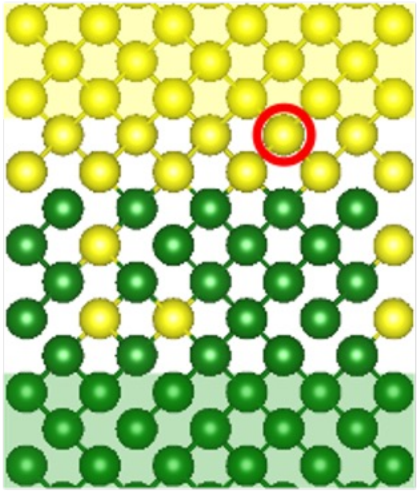
Reverse Model

Extract atomic structures from spectroscopy images



Angle-resolved photo electron spectra (ARPES)





Pimachev and Neogi, arXiv:2302.00261 (2023)

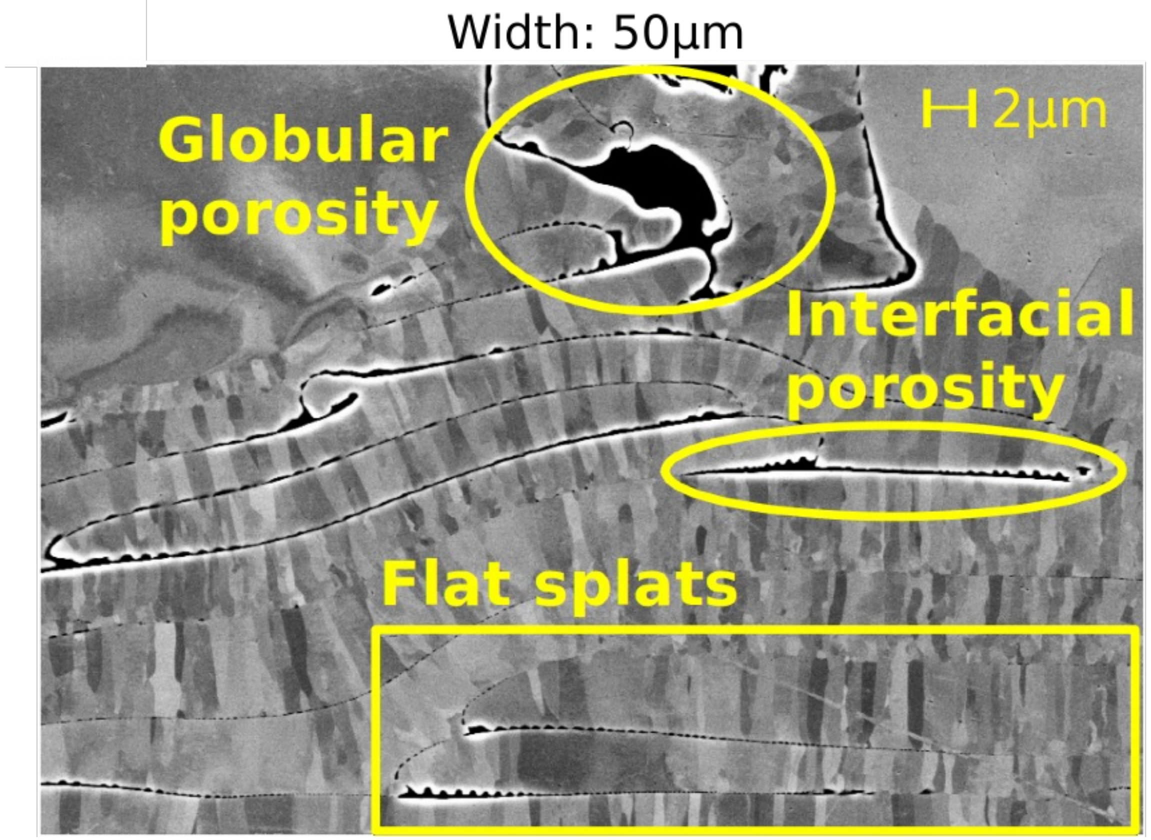
Outline

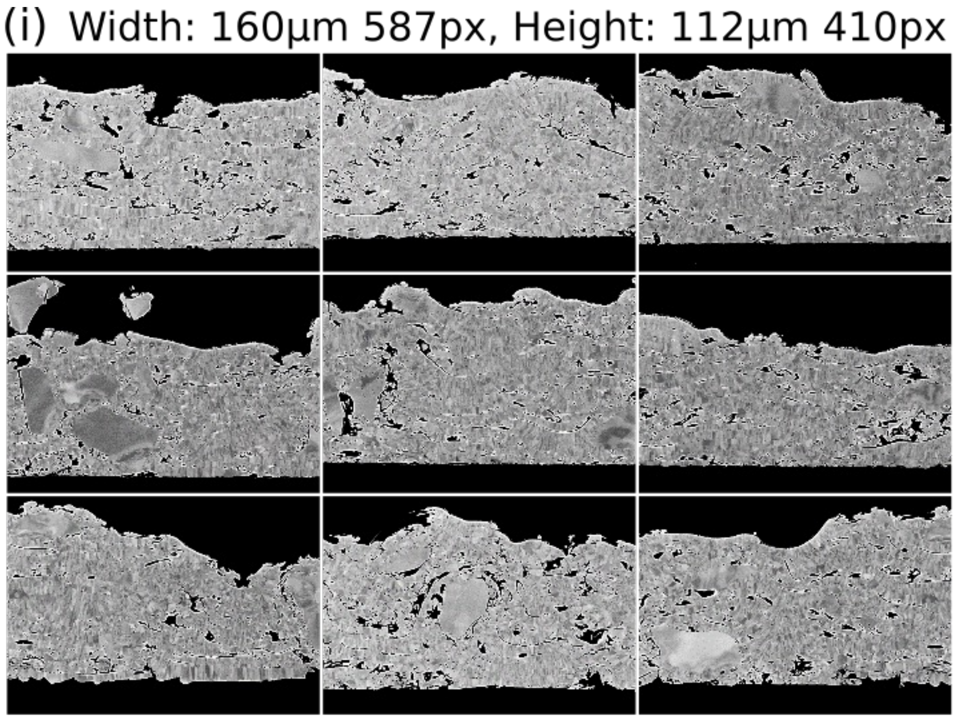
1. Atoms-to-Structures: Electronic Properties of Semiconductor Heterostructures

2. Reverse model: Predicting thermal properties of structural images

Thermal Sprayed Coatings

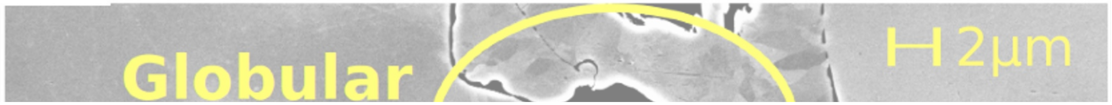
Two-Dimensional (2D) Backscatter Electron Images of Niobium Thermal Spray Coatings





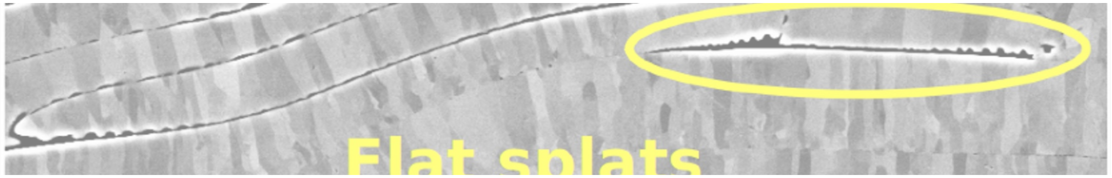
Thermal Sprayed Coatings

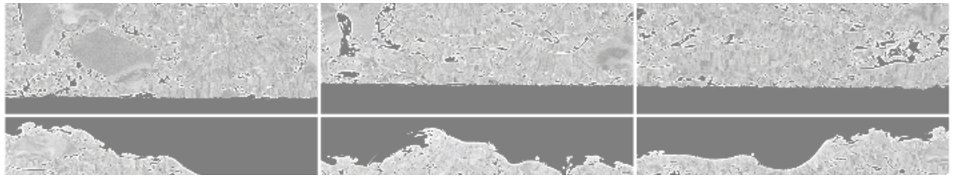
Width: 50µm



(i) Width: 160µm 587px, Height: 112µm 410px

Microscopic structural features that affect thermal properties, eventually durability and lifetime of coatings



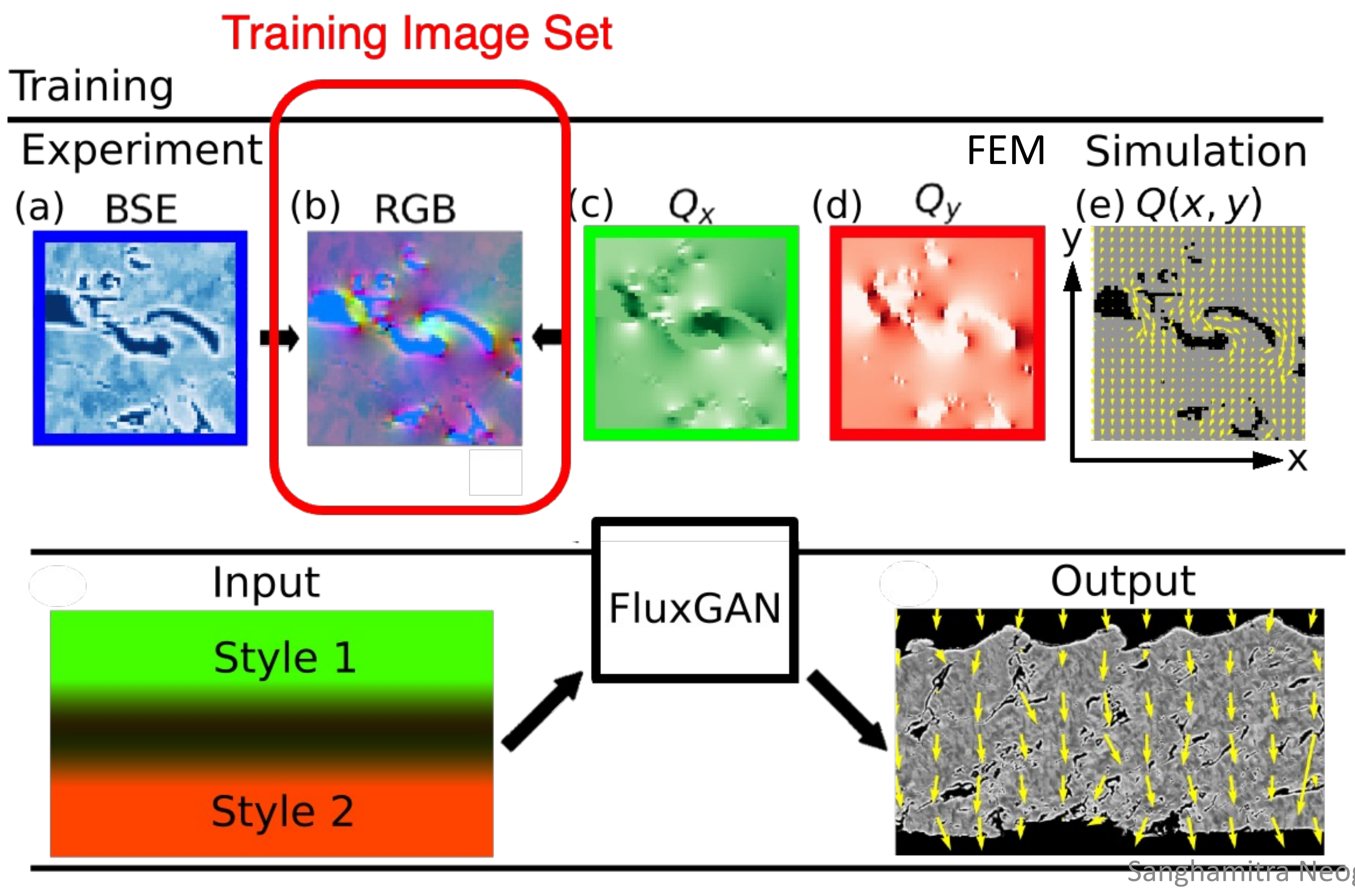


How do different 'classes' of nano-to-microscale features affect thermal properties?

FluxGAN Model

Generates New Coating Images for Input Style Maps

Model Workflow



Training Set

RGB images with channels

Blue: Experimental backscatter electron (BSE) images;
Red: FEM computed top-to-bottom heat flux;
Green: FEM computed left-to-right heat flux;

Augmented with new images obtained by slicing BSE images into smaller images and small rotations

Learning

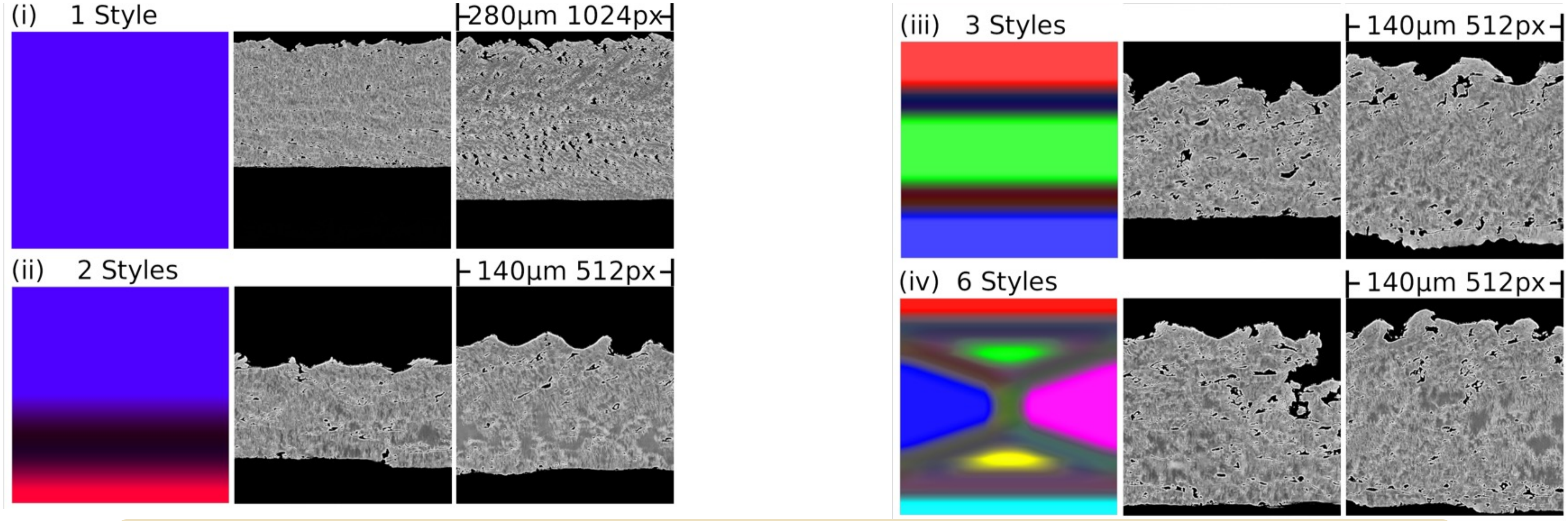
Unsupervised learning of features (styles) in RGB images

Output

Model generates structural images for styles provided as input

Unsupervised Learning of ‘Styles’

Styles $\begin{cases} \text{define different ‘classes’ of nano–to–microscale features of coatings} \\ \text{are closely associated with distribution of heat flux in coatings} \end{cases}$



Styles can be associated with processing parameters

Guided Image Generation for Target Heat Flux

Outpaint

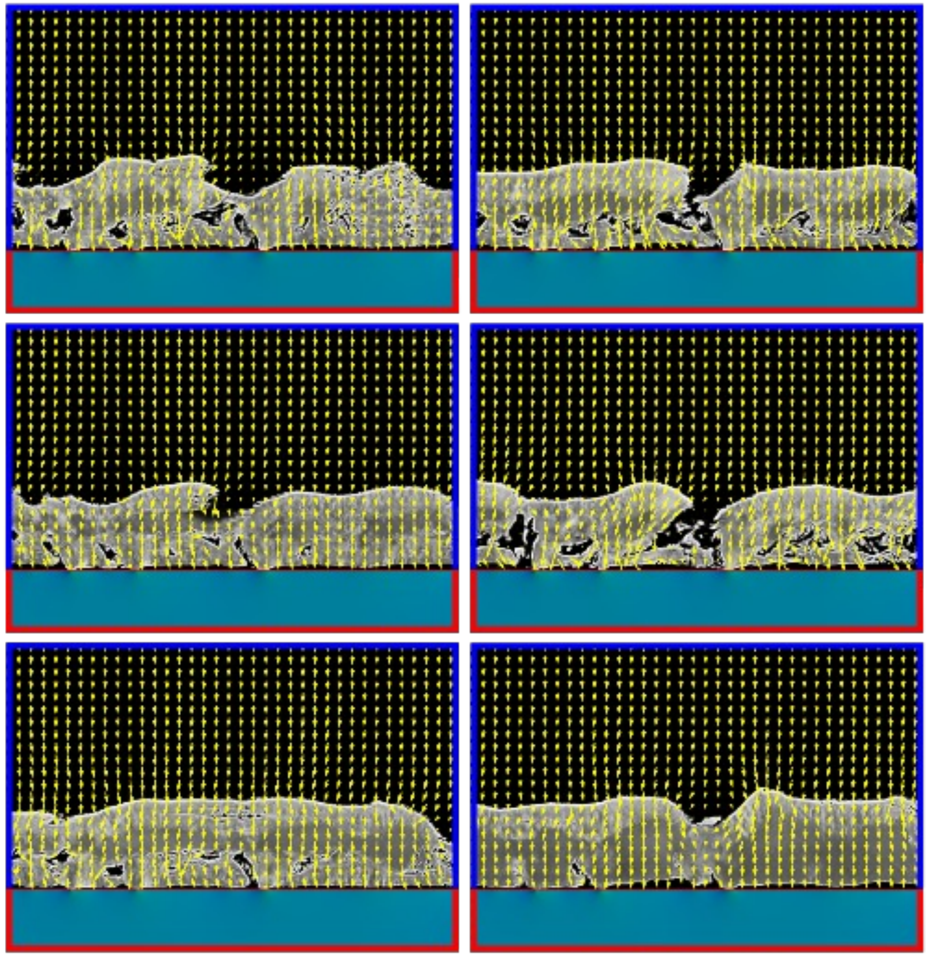
Input

Outpaint

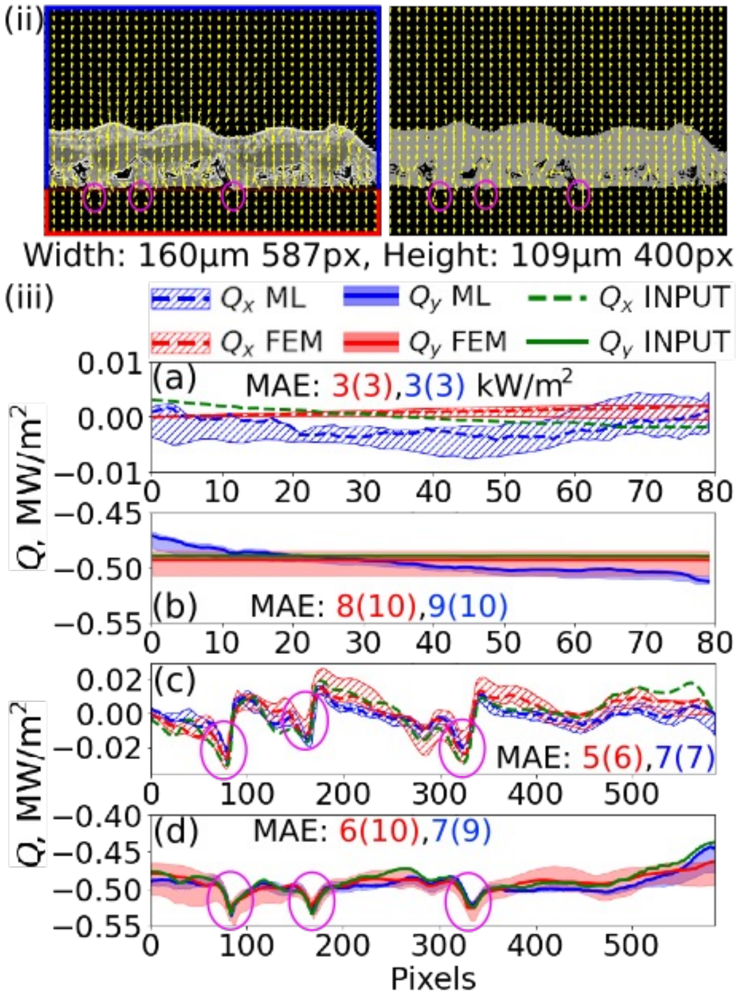
Input

Outpaint

Input

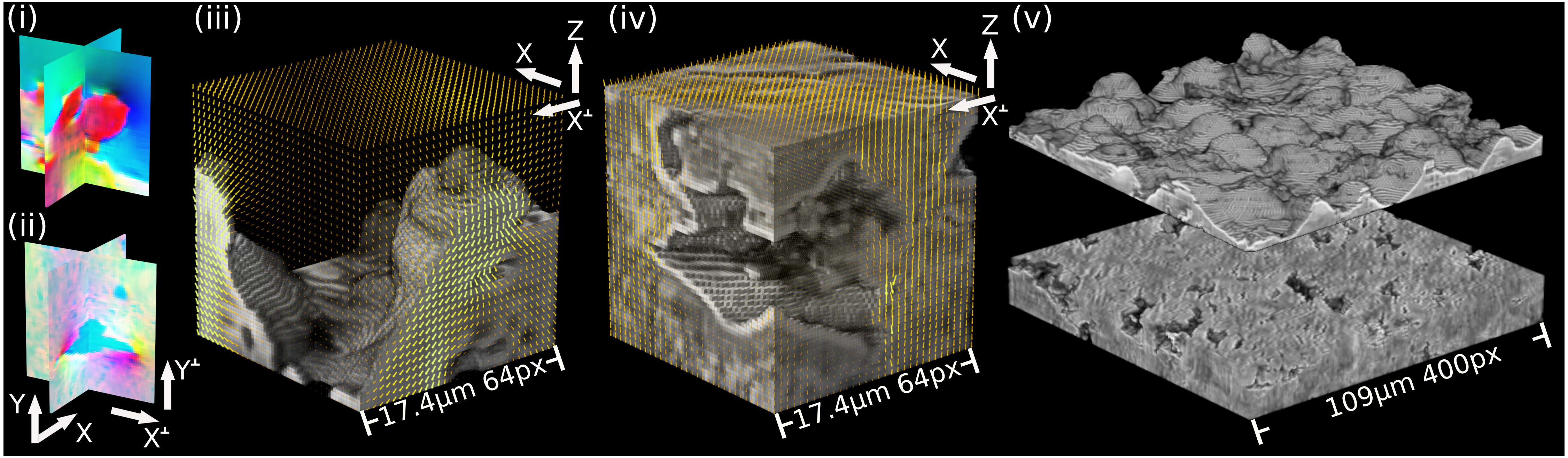


Validation against FEM results



From 2D to 3D

Pimachev, Settipalli and Neogi. arXiv preprint arXiv:2310.04622 (2023)



Provide information about inner structures difficult to access from outside

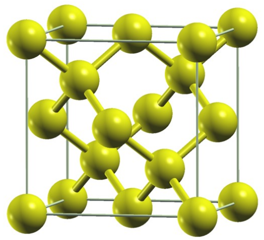
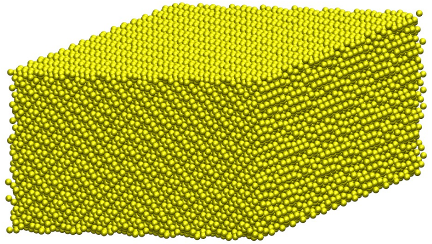
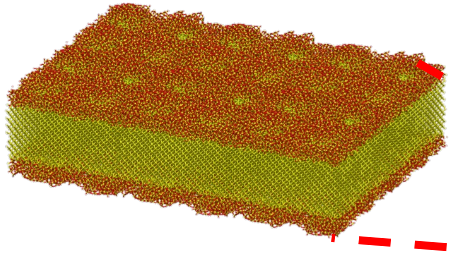
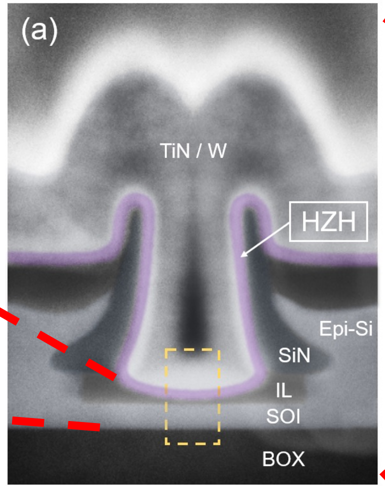
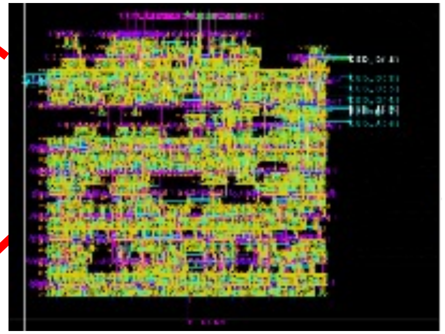
FluxGAN Model

GAN: Generative Adversarial Network

1. is developed using **9** experimental images
2. generates new structures **AND** physical phenomena of interest
3. provides guides for synthesis (e.g., styles created due to spray rate)
4. provides insights to predict materials reliability
5. can be easily generalized to other 2D structures/materials
6. as well as 3D structures

Pimachev, Settipalli and Neogi. arXiv preprint arXiv:2310.04622 (2023)

From Atoms to Devices: Summary

Bulk Silicon	Silicon Channel	Silicon Channel with Insulating Layer	Field Effect Transistor	Chip/Chiplet/Circuit
				

Takeaway messages

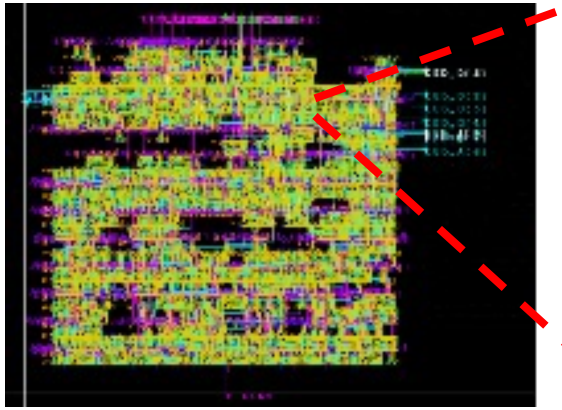
Physics input combined with machine learning approaches can greatly

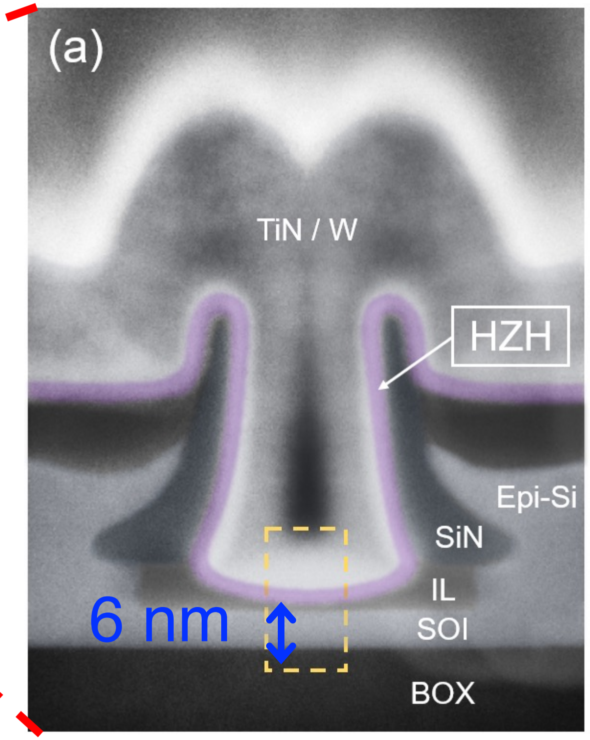
- Facilitate theory-experiment relationship
- Predict materials behavior in complex devices
- Allow application of basic physics knowledge for device design

Thank you!

Back up slides

Atom-to-Circuit Thermal Model of Microelectronic Systems

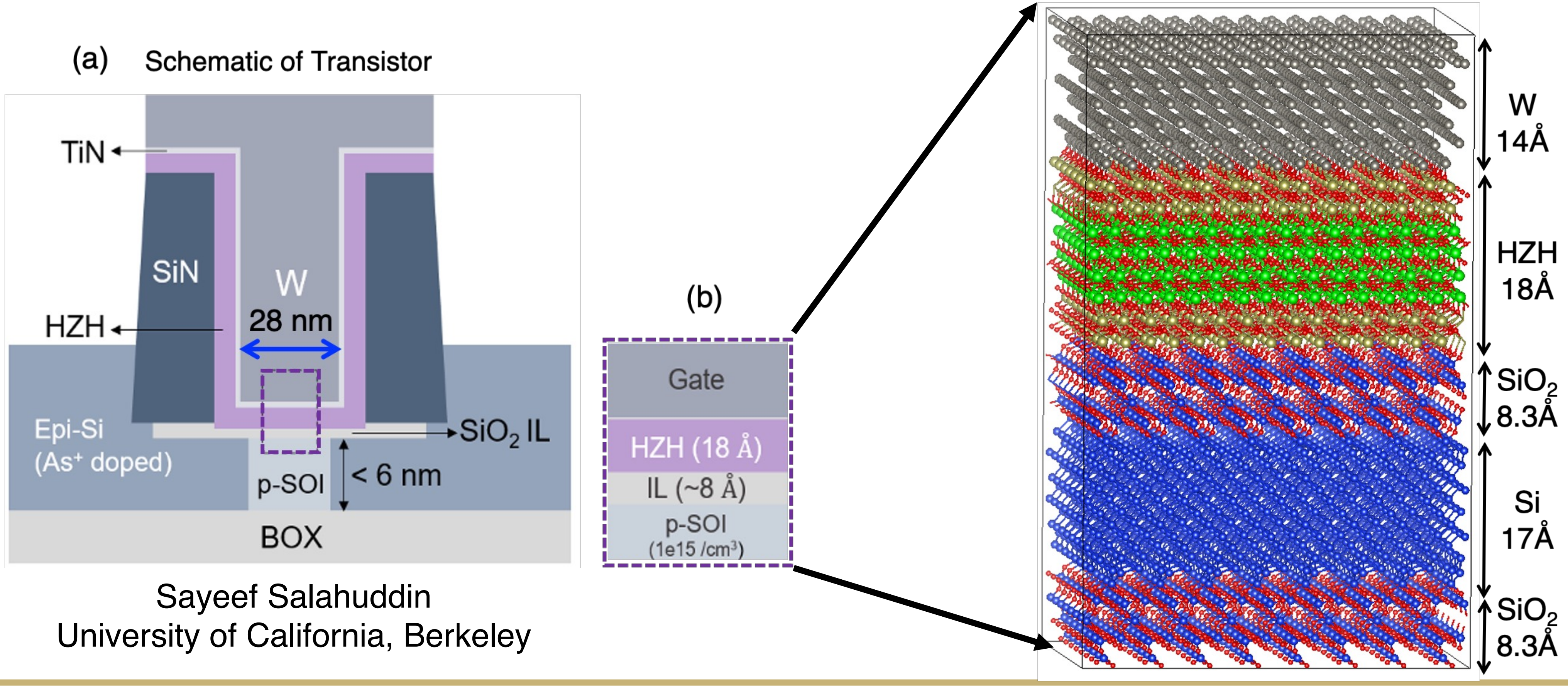




Sayeef Salahuddin
University of California, Berkeley

Bottom Up: Atomistic Model of Transistor

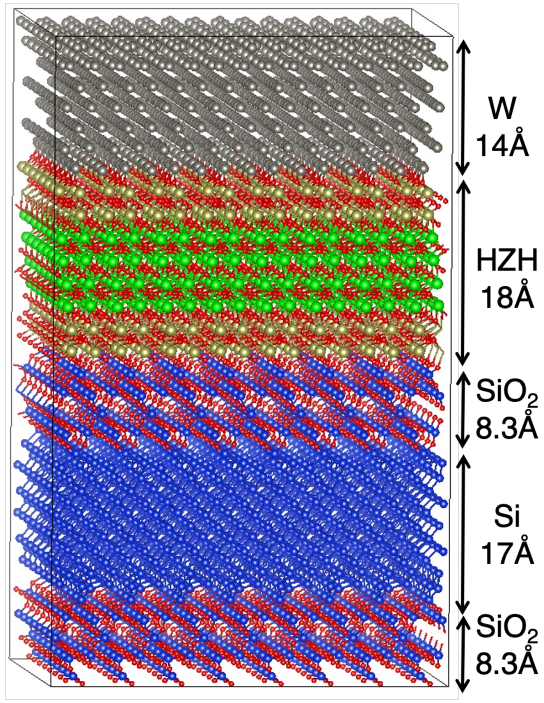
Fully atomistic model of channel region



Sayeef Salahuddin
University of California, Berkeley

Bottom Up: Atomistic Model

Accelerated learning of interactions using GPUs and machine learning (ML) potentials



Training Structures $\xrightarrow[\text{VASP}]{\text{DFT}}$ Reference Forces $\xrightarrow[\text{Fitting}]{\text{GPUMD}}$ Neuroevolutionary Potentials

AI to model interaction potential between atoms

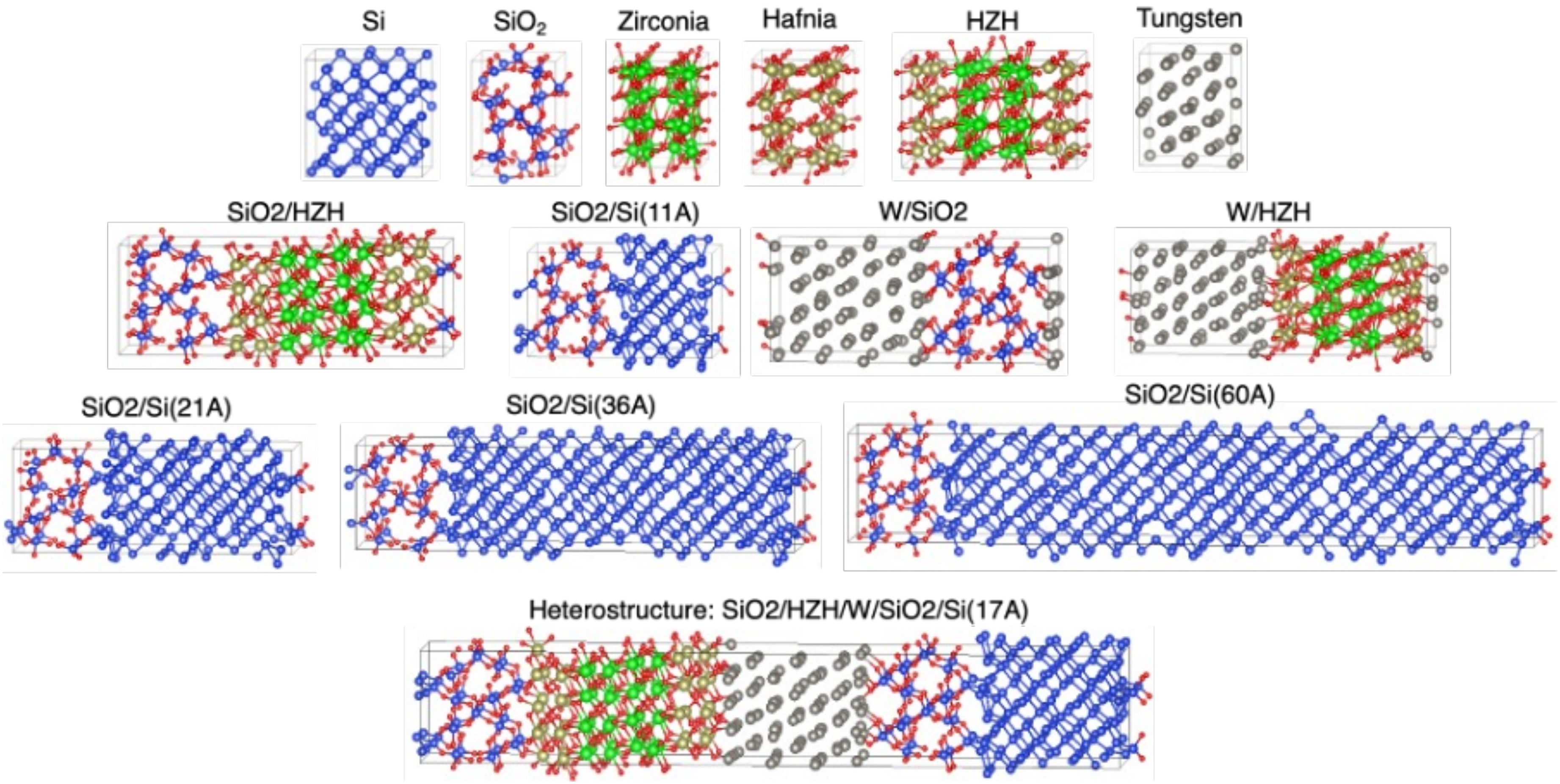
Neuroevolutionary Potentials $\rightarrow$ Relaxed Heterostructure Model $\xrightarrow[\text{Analysis}]{\text{MD}}$ Effective Thermal Resistance

Molecular dynamics (MD) to explore dynamical properties

Sanghamitra Neogi

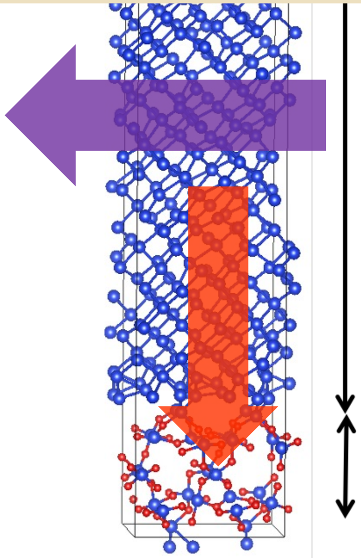
Atomistic Model: Training Data

ML-potential can capture effects due to different channel thicknesses



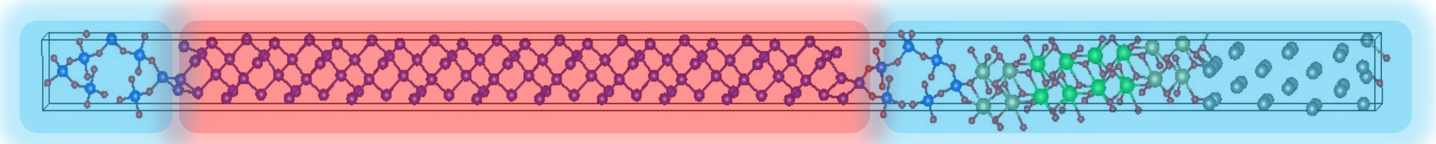
Atomistic Thermal Model: Interfaces

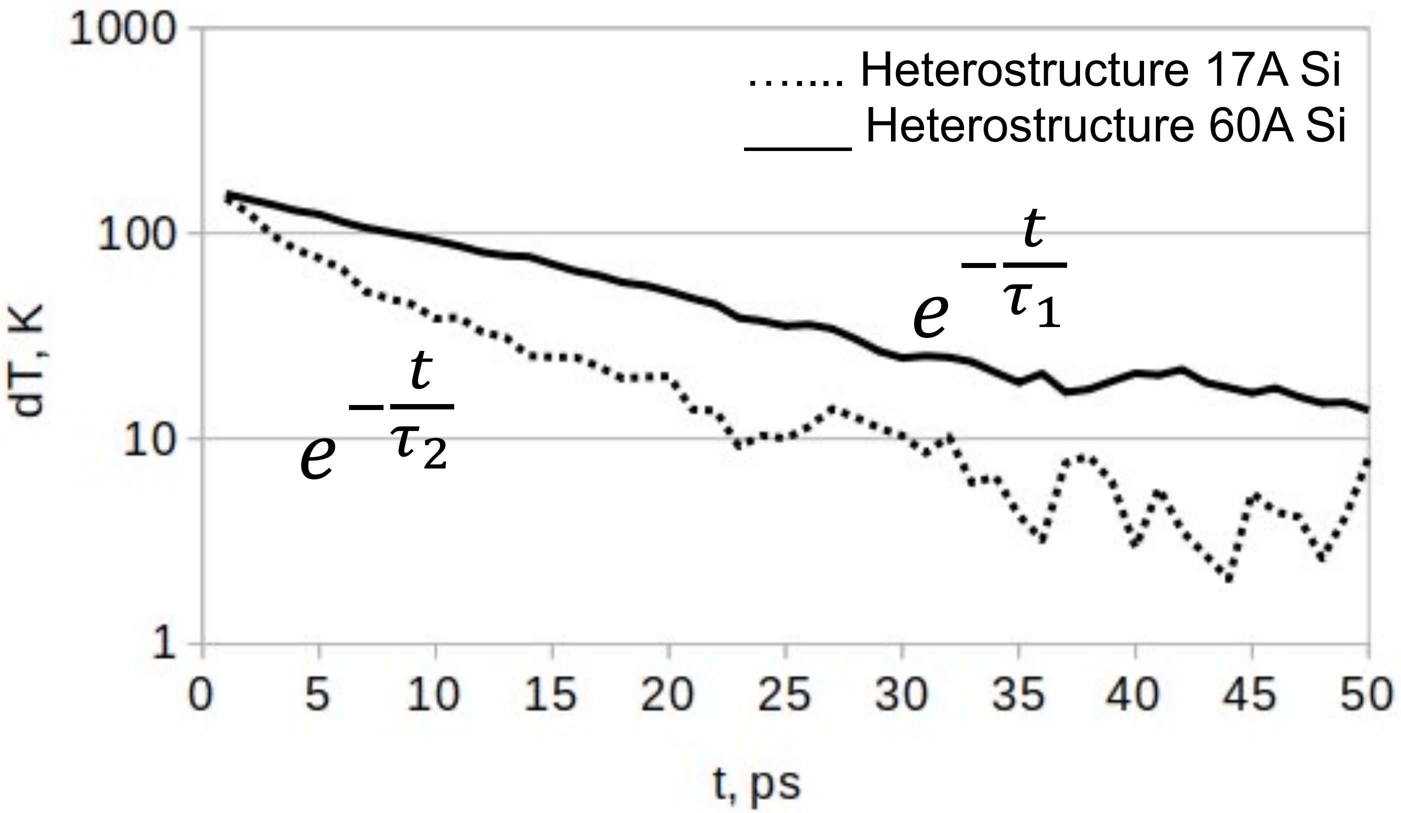
Prediction of thermal bottlenecks in channel region



	Si(6 nm)/ SiO_2(0.85 nm)	Si(3.6 nm)/ SiO_2(0.85 nm)	Si(2.1 nm)/ SiO_2(0.85 nm)	Si(1.1 nm)/ SiO_2(0.85 nm)
Thermal conductivity (cross-plane, W/m-K)	2.39	1.12	0.89	0.68
Thermal conductivity (in-plane, W/m-K)	11.31	8.04	3.50	2.46
Interfacial conductance (GW/m^2-K)	0.768	0.535	0.645	0.751
Interfacial Resistance ($\times 10^{-9}$ m^2-K/W)	1.30	1.87	1.55	1.33

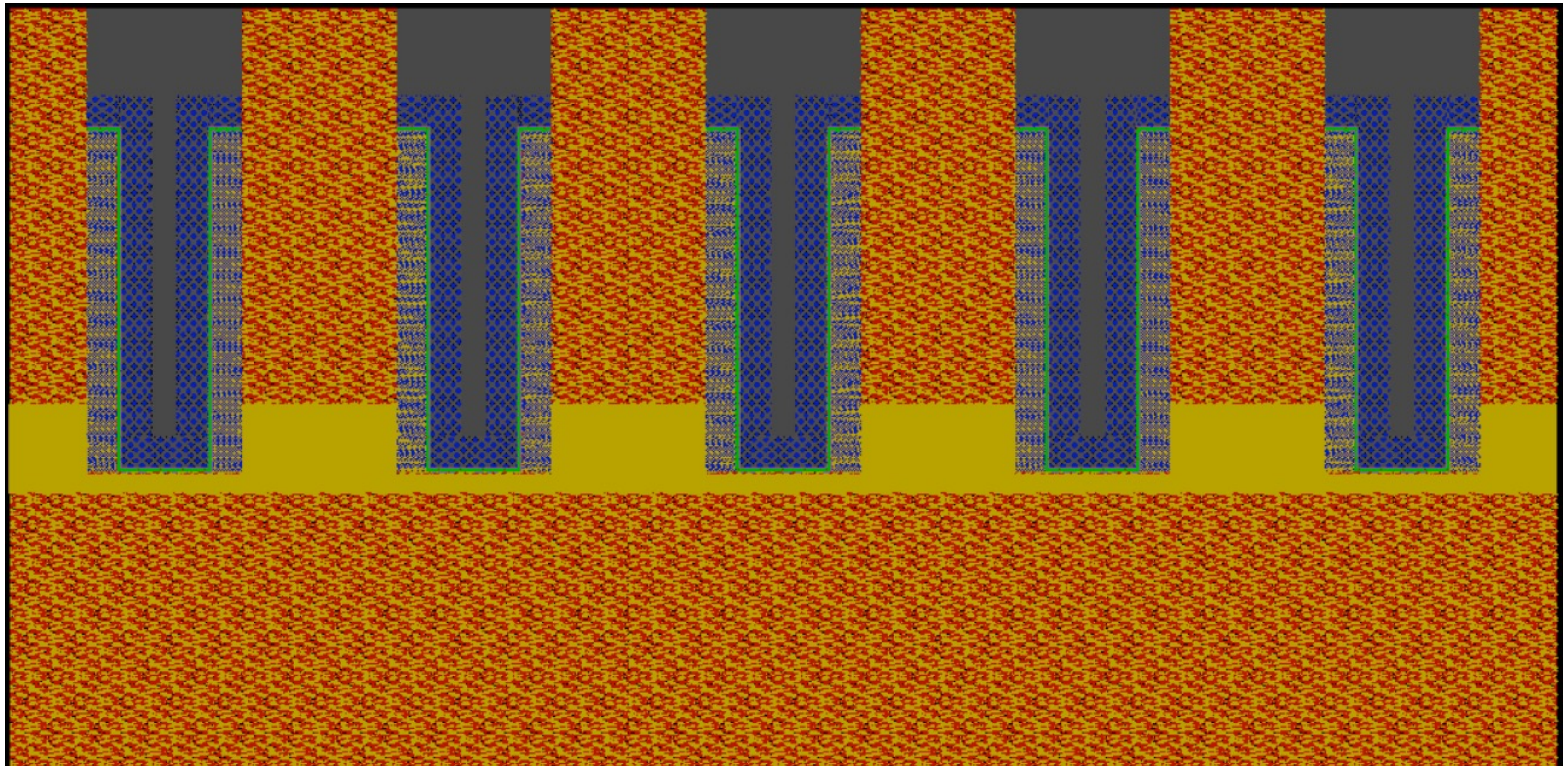
Transient Response



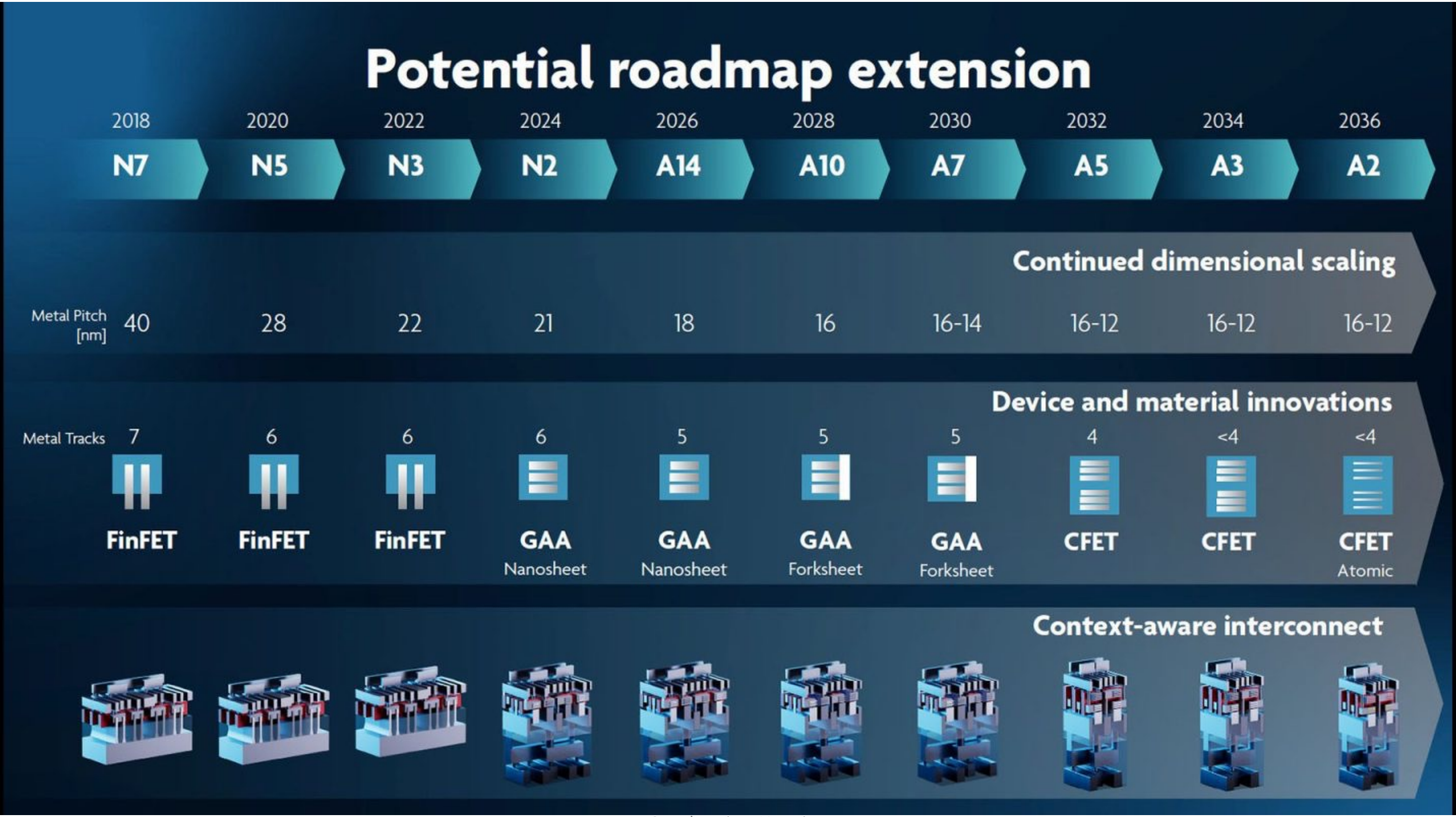


Time-dependent temperature decay due to different Si layer thickness

Next Step: Scaling Up



Steady-state and transient heating dynamics analysis using ML potentials and atomistic molecular dynamics


Potential roadmap extension
2018
2020
2022
2024
2026
2028
2030
2032
2034
2036
N7
N5
N3
N2
A14
A10
A7
A5
A3
A2
Continued dimensional scaling
Metal Pitch [nm]
40
28
22
21
18
16
16-14
16-12
16-12
16-12
Device and material innovations
Metal Tracks
7
6
6
6
5
5
5
4
<4
<4
FinFET
FinFET
FinFET
GAA Nanosheet
GAA Nanosheet
GAA Forksheet
GAA Forksheet
CFET
CFET
CFET Atomic
Context-aware interconnect