Materials in nanoelectronics

EMIRI

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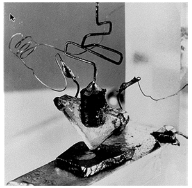
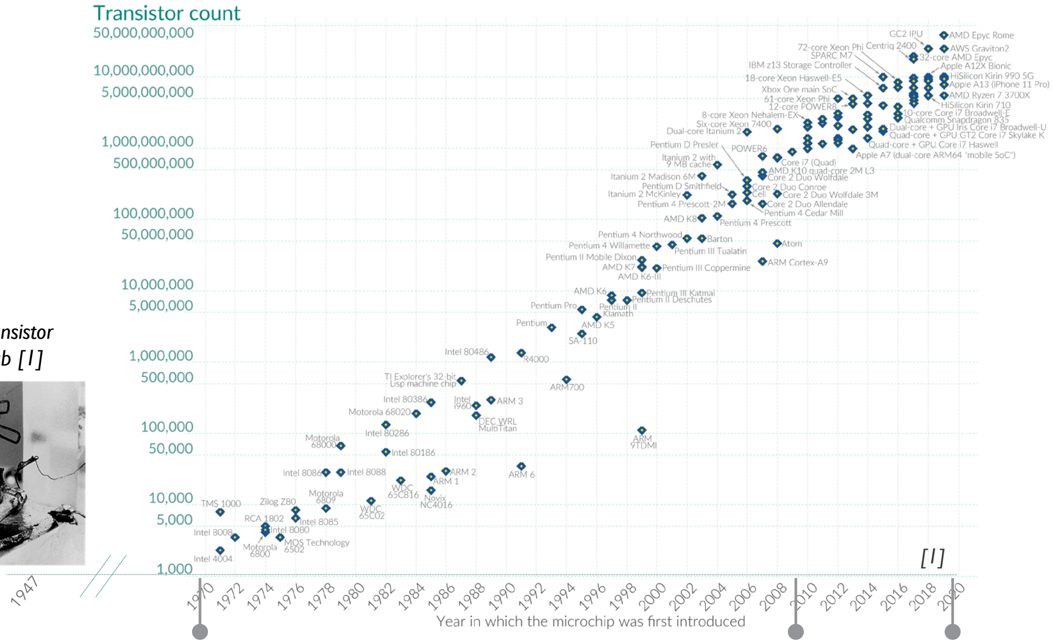
[1] Source: wikipedia.org

Transistor densification in CPU's

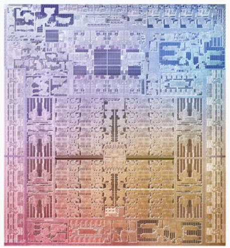
Moore's law

First transistor
Bell Lab [1]





~57x10^{9} transistors



Apple M1 Max (10-cores, 64-bit)

@ human scale:

2300
People, in a conference room

2009:
7.9 billion

1 x

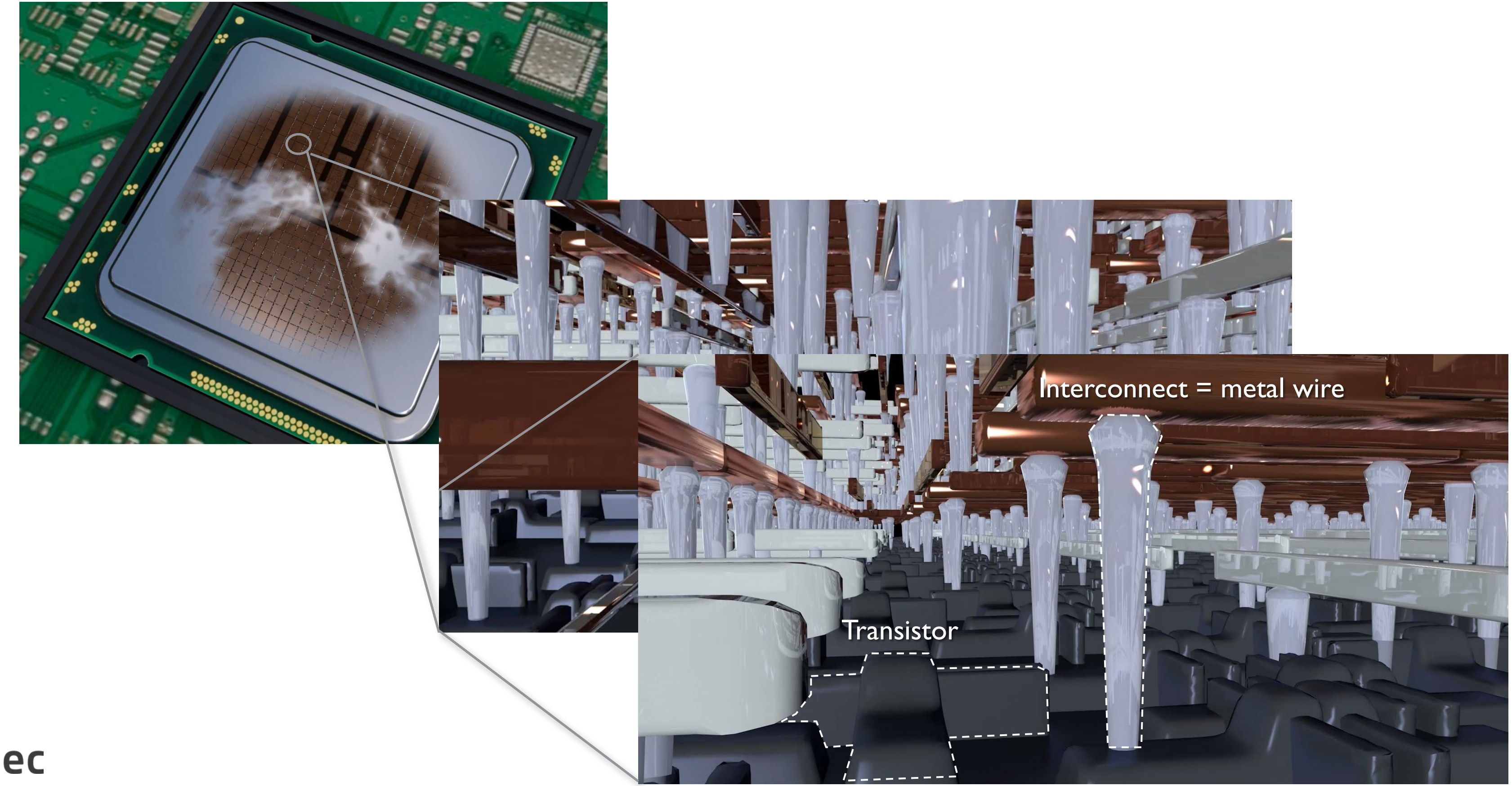
2021:
57 billion

~ 7.2 x

~ 156 x population of US,
~ 7.2 x population of the world
in the same conference room,...

Transistor densification in CPU’s

Imec playground field



Potential roadmap extension

	2018	2020	2022	2024	2026	2028	2030	2032	2034	2036
	N7	**N5**	**N3**	**N2**	**A14**	**A10**	**A7**	**A5**	**A3**	**A2**

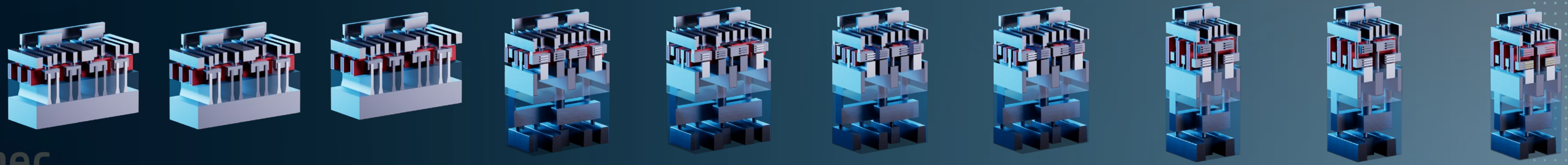
Continued dimensional scaling

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



2025 & data storage about 100ZB/year

1 Zettabyte = 1 billion of Terabytes = 1 trillion of Gigabytes

Transistor densification in CPU’s and memories

INCREASED
PERFORMANCE

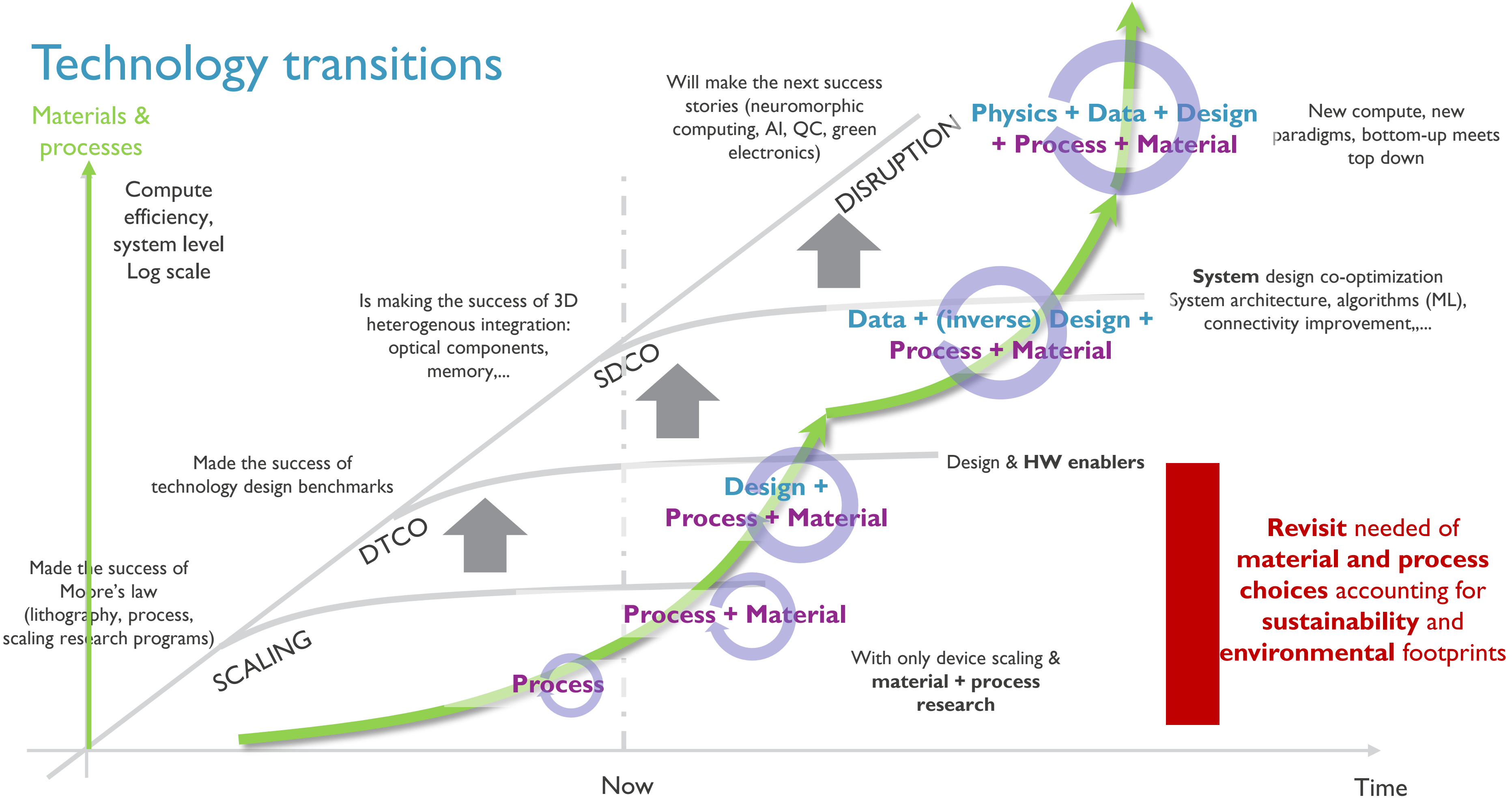
INCREASED
COMPLEXITY

REDUCED
COST

REDUCED
POWER

Driving factors for innovation

Technology transitions



Materials & processes

Compute efficiency, system level Log scale

Made the success of Moore's law (lithography, process, scaling research programs)

Made the success of technology design benchmarks

Is making the success of 3D heterogenous integration: optical components, memory,...

Will make the next success stories (neuromorphic computing, AI, QC, green electronics)

New compute, new paradigms, bottom-up meets top down

SCALING

DTCO

SDCO

DISRUPTION

Process

Process + Material

Design + Process + Material

Data + (inverse) Design + Process + Material

Physics + Data + Design + Process + Material

System design co-optimization System architecture, algorithms (ML), connectivity improvement,,...

Design & **HW enablers**

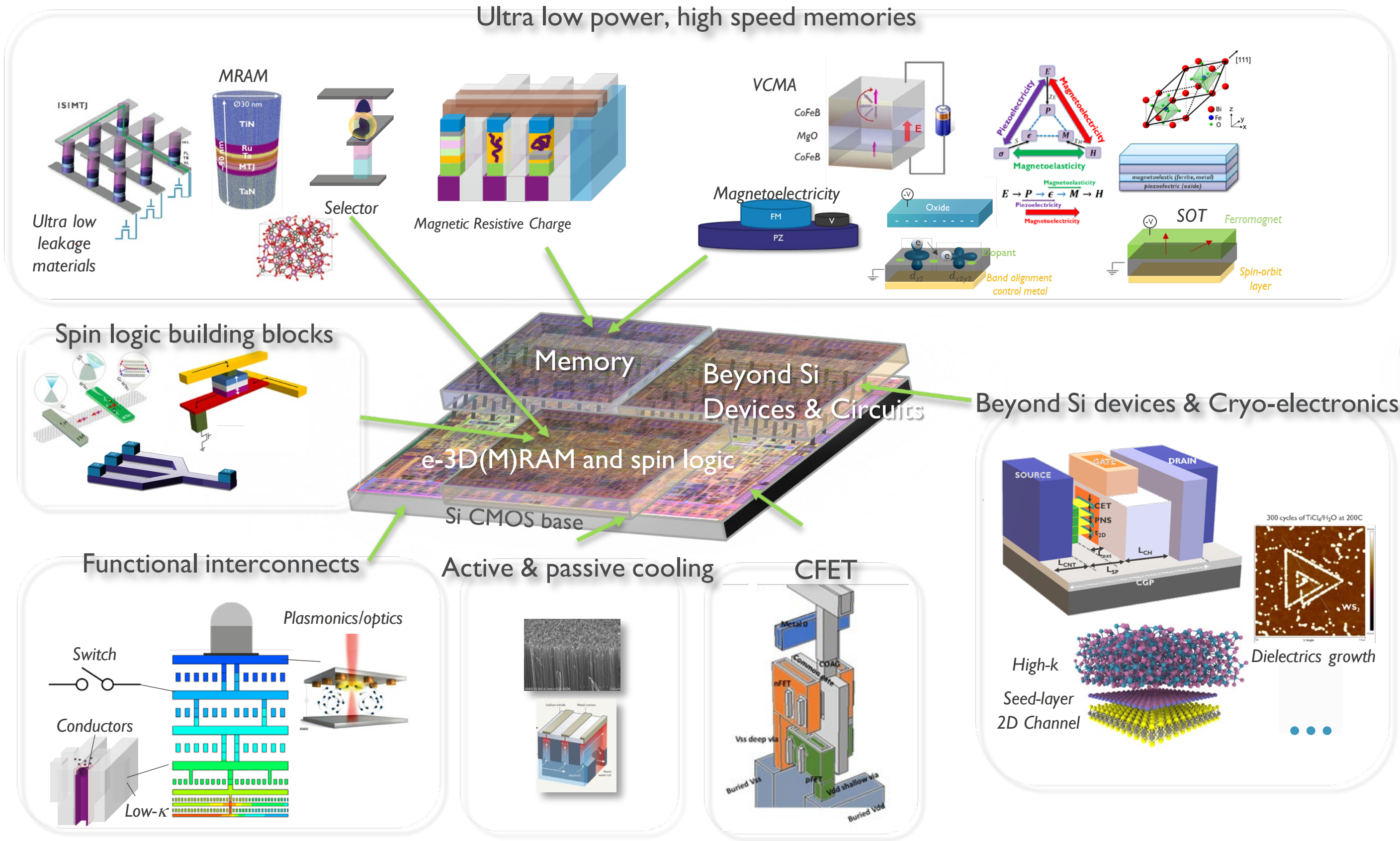
With only device scaling & **material + process research**

Now

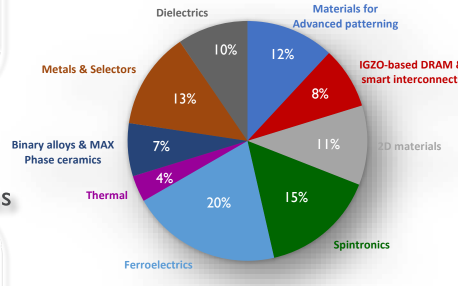
Time

Revisit needed of **material and process choices** accounting for **sustainability** and **environmental** footprints

Speed of learning for material down-selection in their context is critical



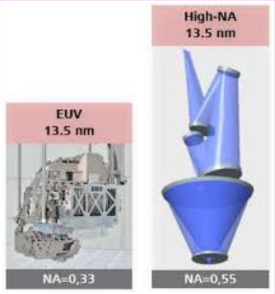
Current projection > 100 potential materials to be evaluated



The future is complex, multi-functional, 3D, and more than ever, material and process dependent....

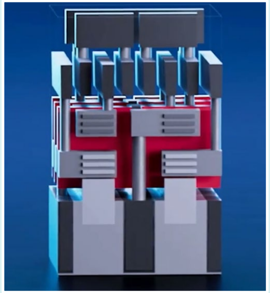
Imec semiconductor technology research pillars

HNA EUV



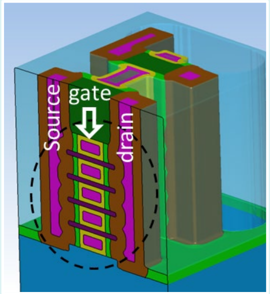
AP3

CFET



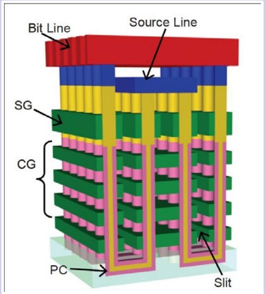
Compute

2D-FET



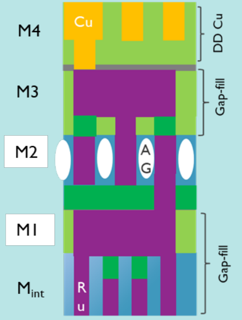
Compute

3D-DRAM



Store

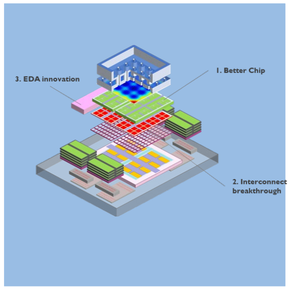
Semidamascene



Semidam Ru M0, M1, M2 AG, M3

Connect

3Di -STCO



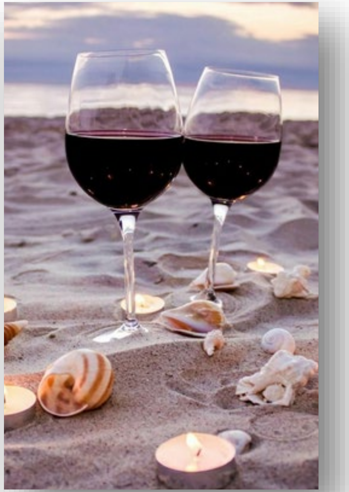
Connect + STCO

Finding the right materials,...

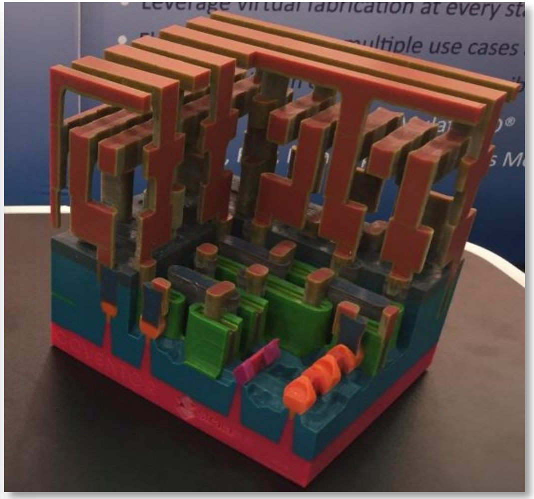
What is the common point between these pictures?

Amorphous SiO_2

Chalcedony spherulites
crypto-crystalline fine-fiber of SiO_2



Amorphous SiO_2



14 nm transistor technology

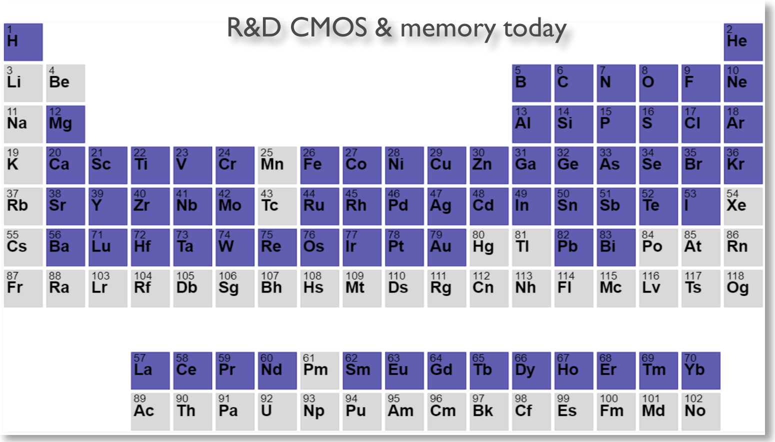
Answers:

- The obvious one: wine
- The less obvious one: SiO_2

1 material = several forms = different functions = different environments

New materials = source of inspiration

But also of perspiration,…



R&D CMOS & memory today

1 H 🟪																	2 He 🟪
3 Li	4 Be											5 B 🟪	6 C 🟪	7 N 🟪	8 O 🟪	9 F 🟪	10 Ne 🟪
11 Na	12 Mg 🟪											13 Al 🟪	14 Si 🟪	15 P 🟪	16 S 🟪	17 Cl 🟪	18 Ar 🟪
19 K	20 Ca 🟪	21 Sc 🟪	22 Ti 🟪	23 V 🟪	24 Cr 🟪	25 Mn	26 Fe 🟪	27 Co 🟪	28 Ni 🟪	29 Cu 🟪	30 Zn 🟪	31 Ga 🟪	32 Ge 🟪	33 As 🟪	34 Se 🟪	35 Br 🟪	36 Kr 🟪
37 Rb	38 Sr 🟪	39 Y 🟪	40 Zr 🟪	41 Nb 🟪	42 Mo 🟪	43 Tc	44 Ru 🟪	45 Rh 🟪	46 Pd 🟪	47 Ag 🟪	48 Cd 🟪	49 In 🟪	50 Sn 🟪	51 Sb 🟪	52 Te 🟪	53 I 🟪	54 Xe
55 Cs	56 Ba 🟪	71 Lu 🟪	72 Hf 🟪	73 Ta 🟪	74 W 🟪	75 Re 🟪	76 Os 🟪	77 Ir 🟪	78 Pt 🟪	79 Au 🟪	80 Hg	81 Tl	82 Pb 🟪	83 Bi 🟪	84 Po	85 At	86 Rn
87 Fr	88 Ra	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
		57 La 🟪	58 Ce 🟪	59 Pr 🟪	60 Nd 🟪	61 Pm	62 Sm 🟪	63 Eu 🟪	64 Gd 🟪	65 Tb 🟪	66 Dy 🟪	67 Ho 🟪	68 Er 🟪	69 Tm 🟪	70 Yb 🟪		
		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No		

- One material = different functions & phases
- 118 space dimensions + process & application dependencies
- And nothing guarantees that the resulting device performances will made it @ the system level

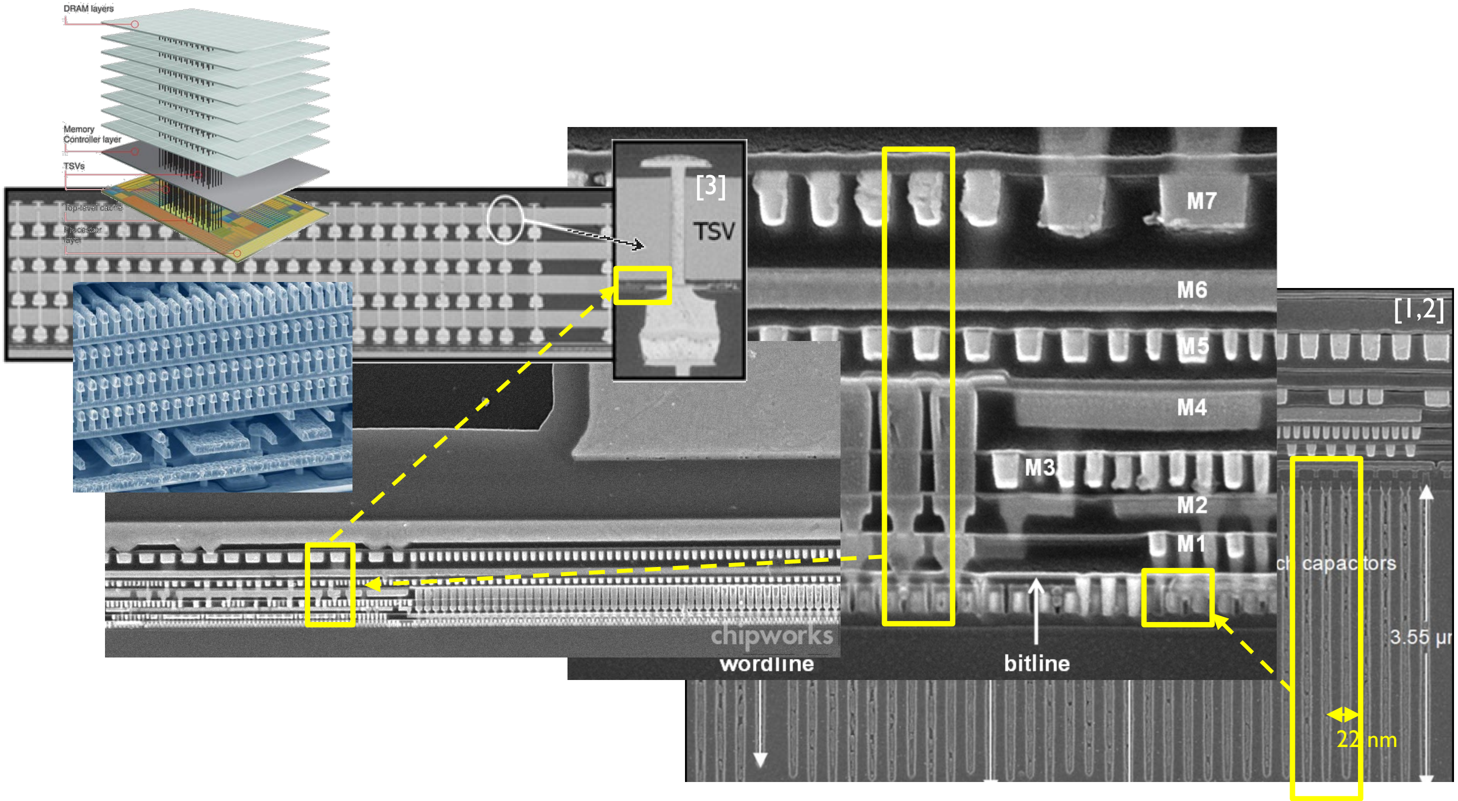
Need "smart" data driven choices of "context aware" materials

[1] http://semimd.com/chipworks/2014/02/07/intels-e-dram-shows-up-in-the-wild/
[2] DRAM: Hybrid memory cube – Micron
[3] e-DRAM-22nm Intel

The structure has become very complex

DRAM

Memory cube 3D stacking [1]

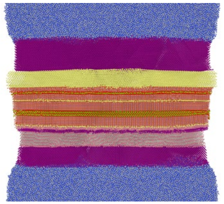


Interfaces start to dominate (< 5nm)

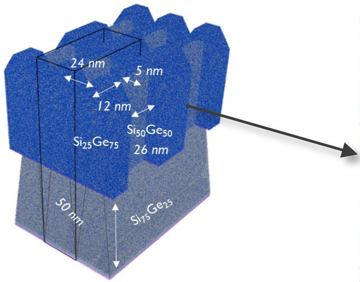
When individual atoms start to matter

- Finite size effects on the electronic structure
- Non-linear behavior of nanometer thick film v.s. bulk
- Interfaces effects start dominating
- Stochasticity plays an important role
- Properties of the stack ≠ sum of isolated materials

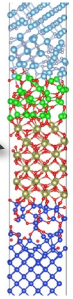
Magnetic RAM multilayered materials

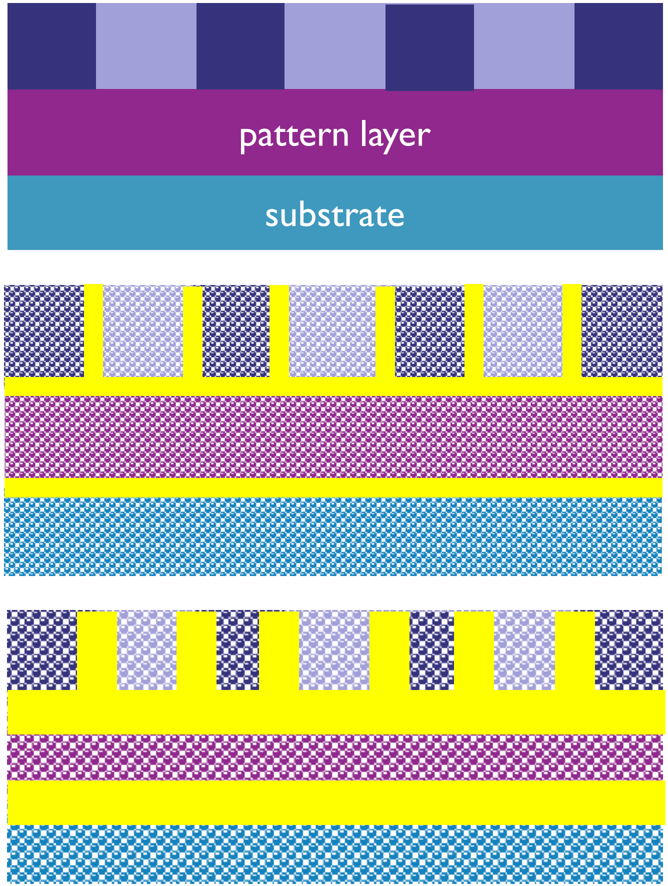


SiGe FinFET's



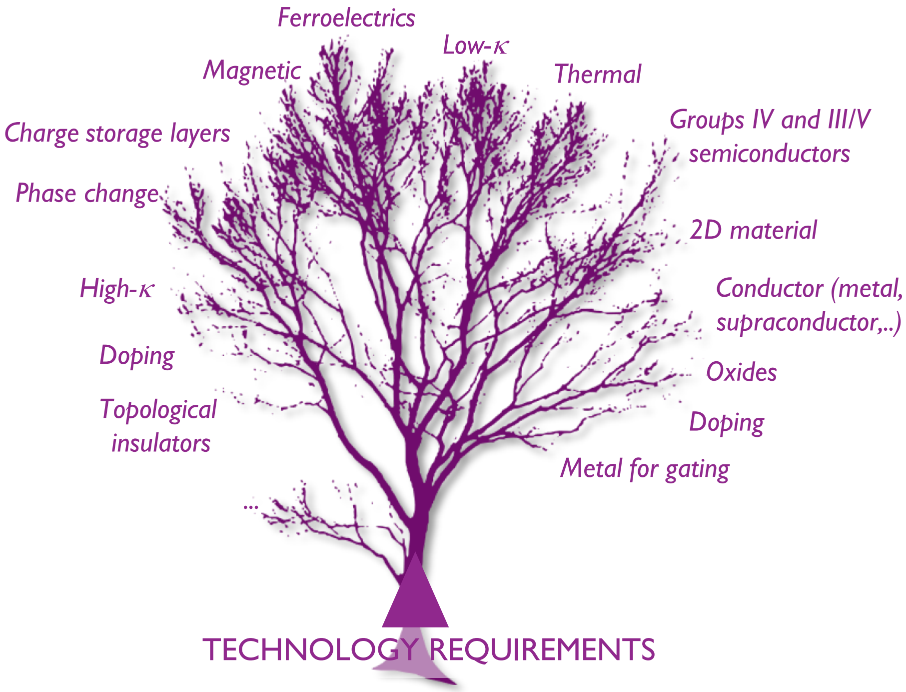
FinFET gate stacks





Material and technology

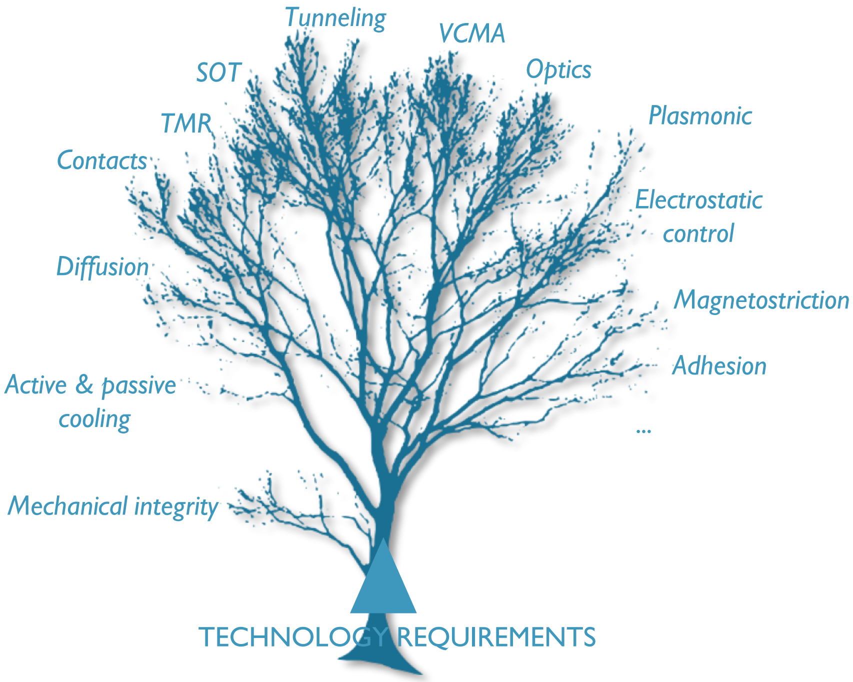
MATERIAL TREE



Ferroelectrics
Low-κ
Magnetic
Thermal
Charge storage layers
Groups IV and III/V semiconductors
Phase change
2D material
High-κ
Conductor (metal, supraconductor,..)
Doping
Oxides
Topological insulators
Doping
Metal for gating
...

TECHNOLOGY REQUIREMENTS

INTERFACE TREE



Tunneling
VCMA
SOT
Optics
TMR
Plasmonic
Contacts
Electrostatic control
Diffusion
Magnetostriction
Adhesion
Active & passive cooling
...
Mechanical integrity

TECHNOLOGY REQUIREMENTS

Challenges:

- Abundancy of reports and of possible solutions
- Confusing literature – no clear benchmarks, results are process and methodology dependent,...
- No clear winner(s)

Material journey:
From concept to 300mm angstrom material pilot line

Material journey: from concept to 300mm angstrom Material pilot line

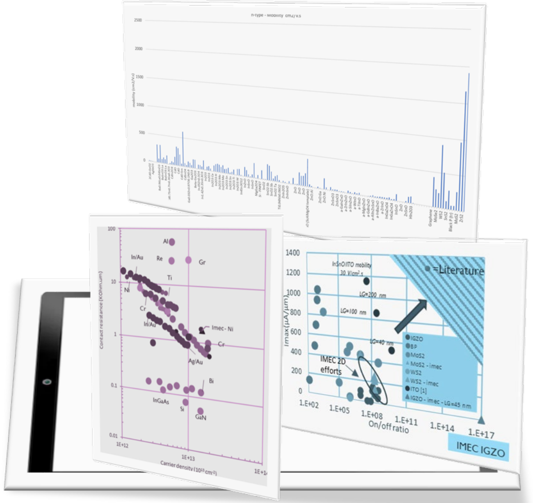
Lab

Virtual & proof of concept

- Define problem & opportunity statement → functional materials
- Data mining : literature screening
- Screening and selection : atomistic & device simulations, lab experiments
- Set-up collaborations with academic centers of excellence

Literature

Data mining



Virtual material screening – ab initio

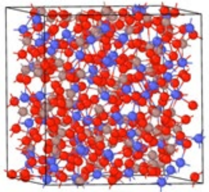
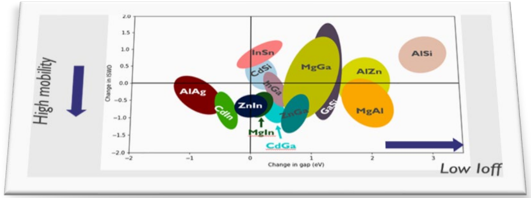


Figure of merits & material selection

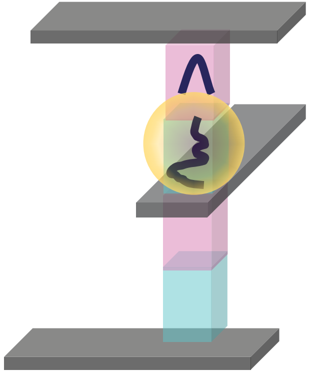


LAB/FAB

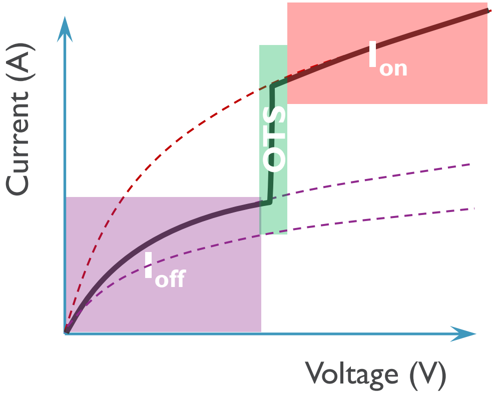
Ex: material requirements for Ovonic Threshold Switch (OTS)

Device specifications

Selector devices



Ideal I.V profile



Device requirements

- Integration , Device & circuit related constraints
  - Current density > 10^7 A/cm^2
  - Non-linearity (NL = I_{on}/I_{off}) > 10^6 @ J_{max}
  - V_{th} > 2 Volts
  - T>400°C

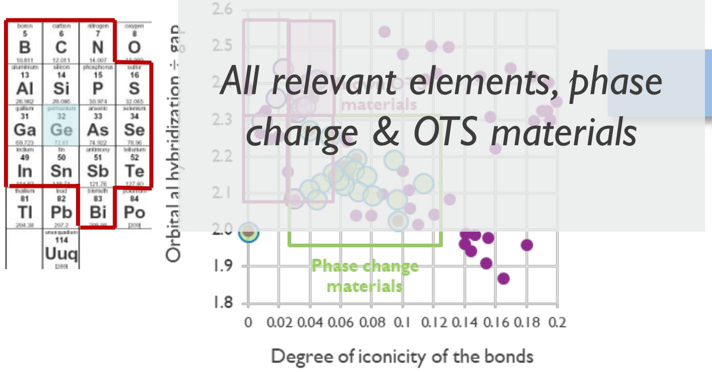
Material requirements

  - Mobility gap ≥ 1.5 eV
  - Low density of defects (10^{19}cm^{-3})
  - $T_{cryst}/T_{melting} \geq 400$ °C
  - Low T deposition, conformality
  - Material thickness min: 4 nm

Material selection for OTS

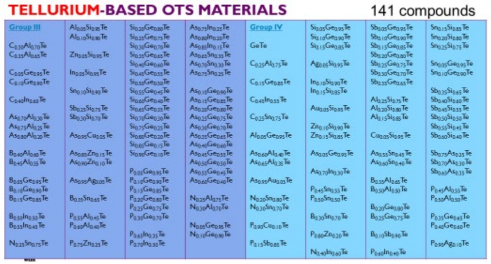
1. Data mining

> 10^6 possible combinations

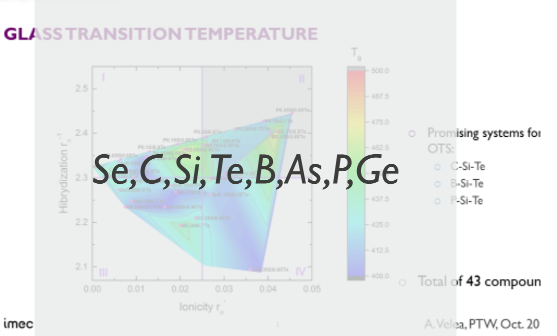


All relevant elements, phase change & OTS materials

2. Down selection

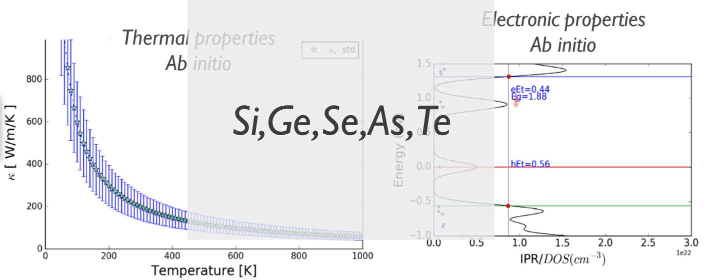

TELLURIUM-BASED OTS MATERIALS

141 compounds



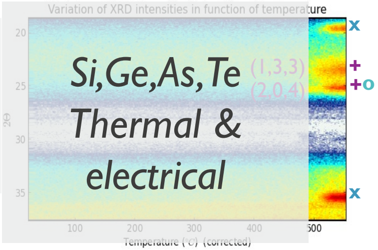
Se,C,Si,Te,B,As,P,Ge

3. Ab initio modeling



Si,Ge,Se,As,Te

4. Material exploration on lab tools

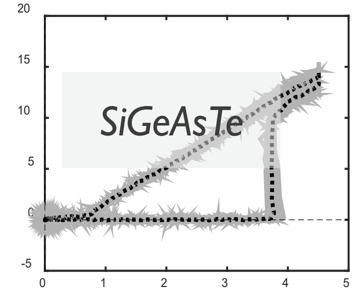


Si,Ge,As,Te
Thermal &
electrical

5. Process development

Precursor selection
Deposition, etch,
integration,...

6. Electrical evaluation



SiGeAsTe

Ex: modeling screening of As/Se-free OTS materials

Identifying materials with tailored electrical properties

1. Element exclusion

As/Se-free ternary compounds consisting of 14 elements (changed by 10% step)

# of valence electrons

2	3	4	5	6
	B	C	N	O
	Al	Si	P	S
Zn	Ga	Ge	As	Se
Cd	In	Sn	Sb	Te

13,104 compositions

2. Glass-transition temperature T_g > 600K

6,596

3. 5 valence electrons 5±0.3

1,490

Ab-initio completed

>1,000

4. Stability E_{form}<0

5. Leakage ΔE_t>0

360

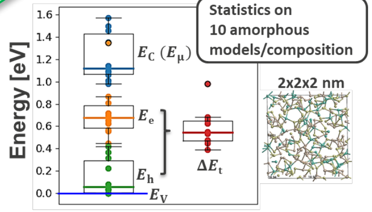
6. Target window $E_\mu - \Delta E_t$

26

12

7. OTS gauge >18

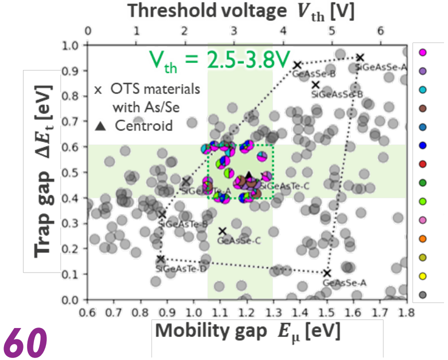
8. Phase stability $T_{spinodal}$ < 0°C



Statistics on 10 amorphous models/composition

e.g. $S_{0.5}Ge_{0.1}Sn_{0.4}$

Selector for RRAM



Promising candidates

OTS gauge

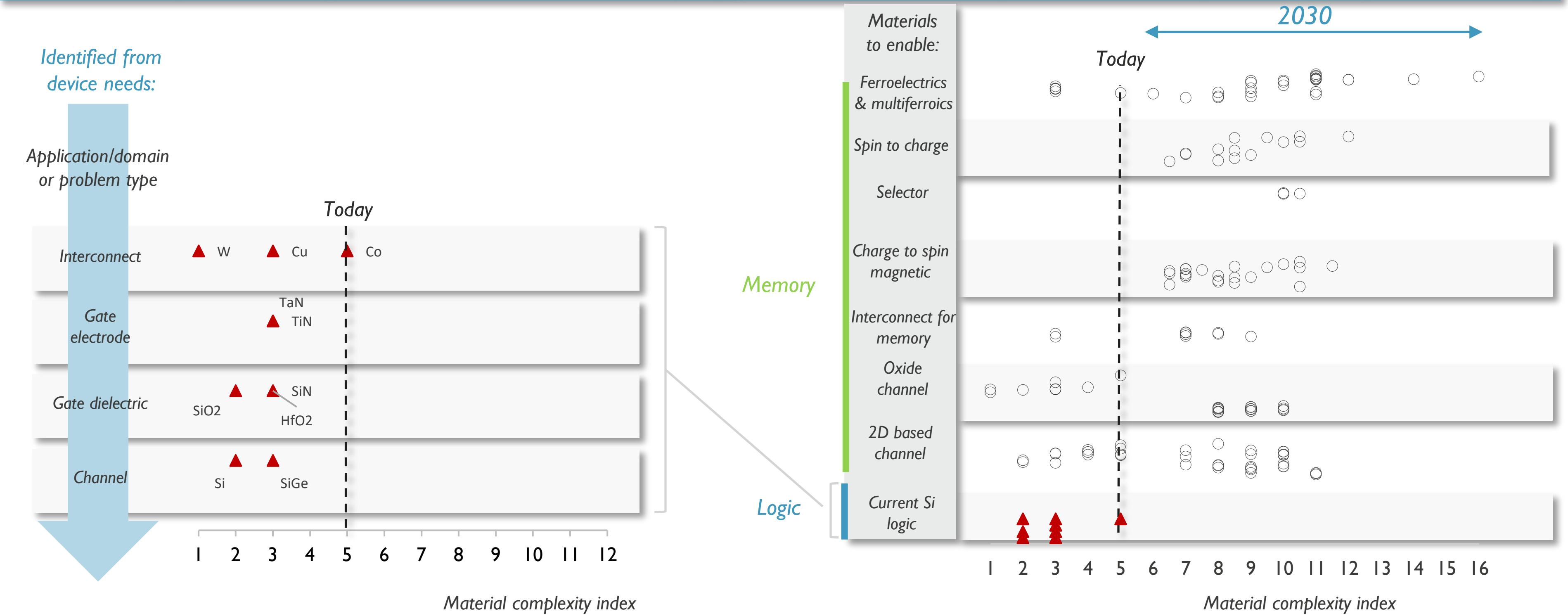
12 Promising candidates identified → M&ILAB

Material index

Contextual guidance for material selection

Step function:
0 = no problem
1 = problematic

Index = <# Elts/layer> + Oxid. stage + Int. switch + Adhesion + Etch + Quality growth T < 400°C + Reactivity + Phase + Ease of deposition + Env. Impact + Conformality



Gap analysis: material screening, in-situ interface control, etching and advanced physical characterization are keys

Material journey: from concept to 300mm angstrom Material pilot line

Lab

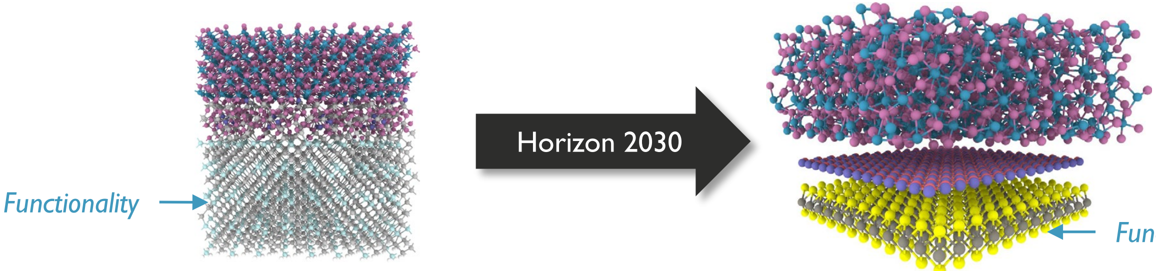
Virtual & proof of concept

- Define problem & opportunity statement → functional materials
- Data mining : literature screening
- Screening and selection : atomistic & device simulations, lab experiments
- Set-up collaborations with academic centers of excellence

Lab2Fab Attolab,
M&I Lab + Lab

Phase I : Explore

- Screening : identify materials with tailored properties
- Processing : definition of process windows
- Understanding : impact of interfaces
- Specs for alpha tool development
- Explore compatibility with integration (passive materials & corrosive gasses)



2020: device steered by bulk

2030+ : device steered by interface

"The interface is the device" (Herbert Kroemer)

"God made the bulk, the surface was invented by the devil" (Wolfgang Pauli)

Bulk material properties ≠ thin film properties

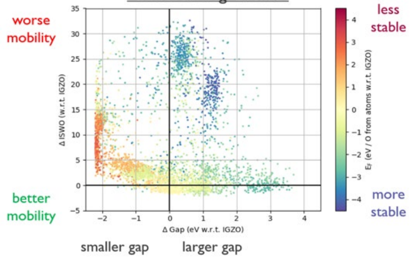
Stack properties ≠ Σ thin film properties → Σ (interface + material)

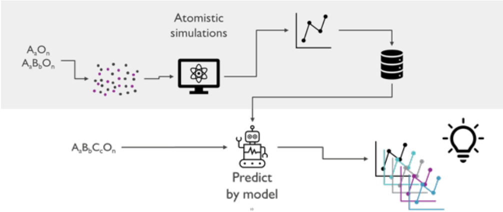
Methodology for accelerated material developments

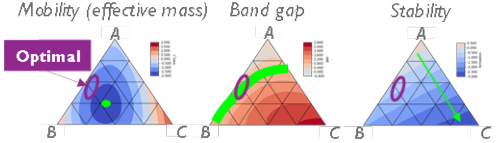
6 digits .... of possible combinations

Ab initio simulations

Full screening dataset

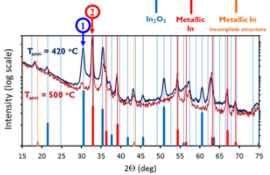




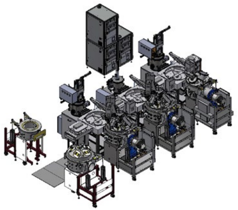


Ab-initio and ML-based shortlist Functional materials

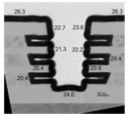
2 digits of potential new materials

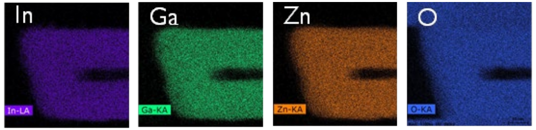


Process clustering @ lab scale



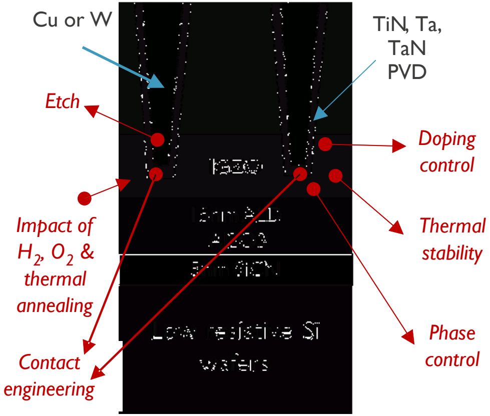
- \+ Interfaces increasingly important (study diffusion, avoid air exposure)
- \+ Small precursor volumes
- \+ PVD, ALD, metrology
- \+ e-beam, lithography

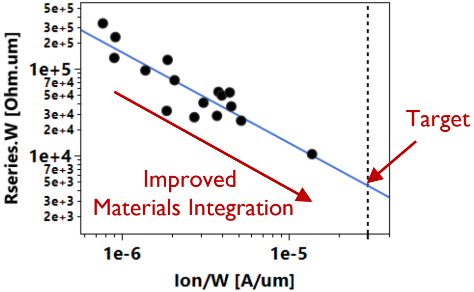




Fast, coupon level elimination

1 digit in the FAB

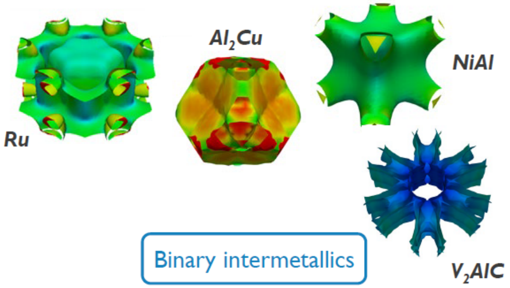


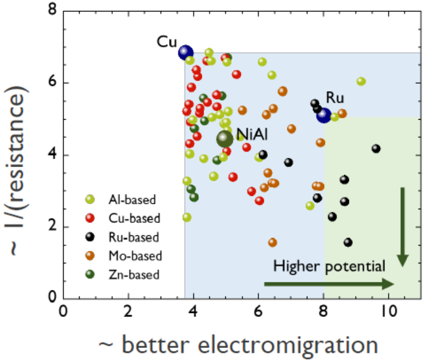


300mm modules & integration

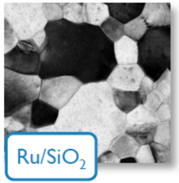
Accelerated development of new conductor materials

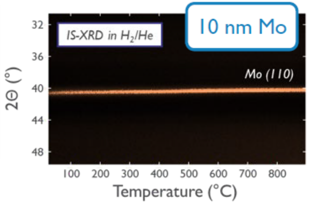
Ab initio calculation of electronic structures





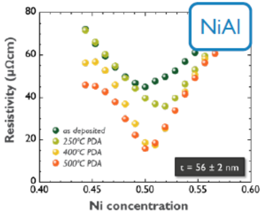
Ab-initio-based shortlist

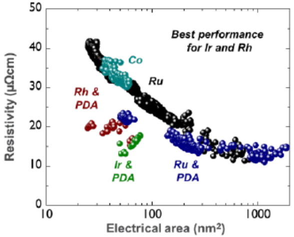




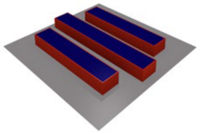
Thin film characterization:

- Resistivity
- Crystalline phase
- Grain size
- Recrystallization
- Chemical inertness
- Adhesion and stress





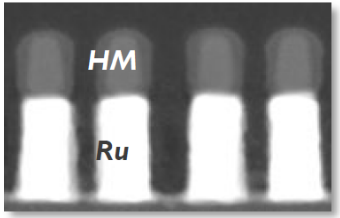
Short-loop line resistance



Metal spacer process

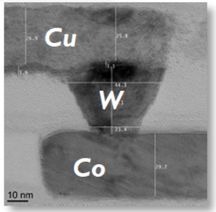
Thin film and short-loop evaluation

Ru semidamascene module: (deposition, RIE, clean)



Ru lines by subtractive etching

Hybrid metallization module: (deposition, CMP, clean)



Wet cleaning of binary metals

	Etch rate (nm/min)	
	NiAl	**Al_3Sc**
0.05% HF	7.2	> 44
1.45% NH_4OH	0.3	0.06
APM	4.5	0.3

300mm modules & integration

Material journey: from concept to 300mm angstrom material pilot line

Lab

Virtual & proof of concept

- Define problem & opportunity statement → functional materials
- Data mining : literature screening
- Screening and selection : atomistic & device simulations, lab experiments
- Set-up collaborations with academic centers of excellence

Lab2Fab

Phase 1 : Explore

- Screening : identify materials with tailored properties
- Processing : definition of process windows
- Understanding : impact of interfaces
- Specs for alpha tool development
- Explore compatibility with integration (passive materials & corrosive gasses)

Lab2FAB + Fab : hybrid process modules

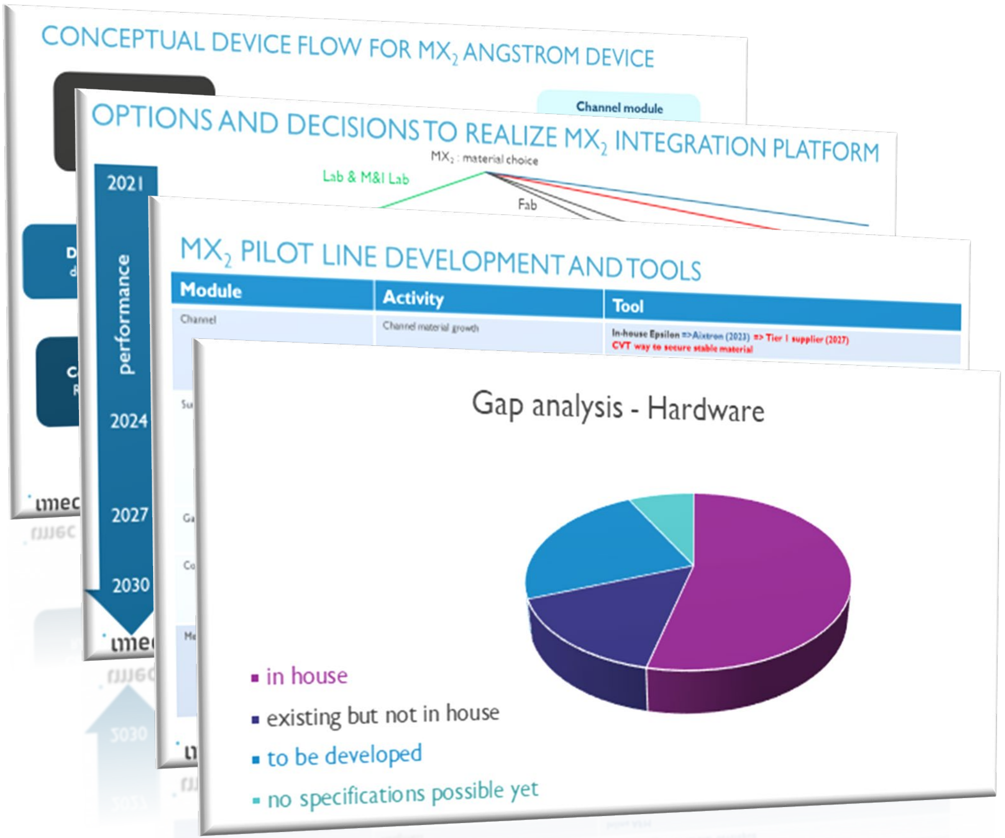
Phase 2 : Pathfinding

- Ecosystem : co-develop materials with suppliers
- Upscale defined process windows to 12 inch
- Demonstration of generic modules in 12 inch
- Alpha tool development (JPD)

"One time right"
introduction in 300mm Fab

Criterion for the selection of materials does not come through properties only : constraints bound to integration schemes & processes for module development also need to be accounted for

Methodology to define project infrastructure : gap analysis



CONCEPTUAL DEVICE FLOW FOR MX$_2$ ANGSTROM DEVICE

OPTIONS AND DECISIONS TO REALIZE MX$_2$ INTEGRATION PLATFORM

MX$_2$ PILOT LINE DEVELOPMENT AND TOOLS

Module	Activity	Tool
Channel	Channel material growth	In-house Epsilon =>Aixtron (2023) => Tier 1 supplier (2027) CVT way to secure stable material

Gap analysis - Hardware

- in house
- existing but not in house
- to be developed
- no specifications possible yet

- Conceptual process flow :
  - Complex & convoluted problem
  - Key questions & minimal spec definition

- Deconvolution into problem statements
- Strategy to tackle different key problems :
  - Gate stack, contact, doping strategy,...

- Target :
  - 300mm tool specifications

- List of equipment needs and specs for device demonstration :
  - In house tools
  - Gap definition
    - Existing tools (not in house)
    - Tools to be developed (engagement with tool suppliers)
    - Metrology needs

Development Phases of 300 mm angstrom Material pilot line

Lab

Virtual & proof of concept

- Define problem & opportunity statement → functional materials
- Data mining : literature screening
- Screening and selection : atomistic & device simulations, lab experiments
- Set-up collaborations with academic centers of excellence

Lab2Fab Attolab,
M&I Lab

Phase 1 : Explore

- Screening : identify materials with tailored properties
- Processing : definition of process windows
- Understanding : impact of interfaces
- Specs for alpha tool development
- Explore compatibility with integration (passive materials & corrosive gasses)

Lab2FAB + Fab: hybrid process modules

Phase 2 : Pathfinding

- Ecosystem : co-develop materials with suppliers
- Upscale defined process windows to 12 inch
- Demonstration of generic modules in 12 inch
- Alpha tool development (JPD)

Fab-pilot line: Integrated device

Phase 3: development

- Development of production tool
- Demonstration of integrated product
- Pilot line : beta tools (tier1&2 vendors)

Production

Investment ~2.5B€

Guided tour next

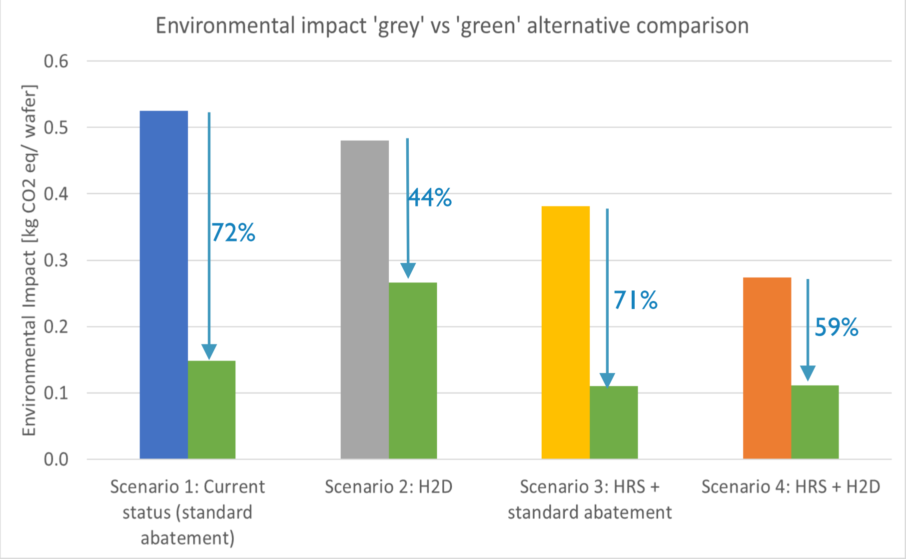
Electronic industry = ~ 4% world CO_2 emission

Can imec contribute to the reduction of the footprint ?

GWP= Global warming potential

Ex: hydrogen circularity in EUV lithography at imec

- H_2 is essential for EUV scanner functionality
- H_2 has a relatively high GWP_{100} factor of 12.8*
- Initial test for recycling hydrogen at imec in 2022
  - No adverse effects observed on scanner
  - H_2 consumption reduced by 70%
    - Anticipate 80% reduction in the future
- Life Cycle Analysis (LCA) applied to quantify benefit
  - 4 scenarios modelled using primary material flow data from Edwards
    1. Standard abatement (combustion with natural gas)
    2. H_2D (H_2 dilution with air before direct emission)
    3. HRS + standard abatement (H_2 recycling & combustion)
    4. HRS + H_2D (H_2 recycling & H_2 dilution)
- A sensitivity analysis was done to access the impact of reducing the electricity carbon intensity and using a non-fossil-based source of H_2



Results

- H_2 dilution results in the smallest reduction of environmental impact in comparison to standard abatement. Due to H_2 contributing to scope 1 emissions.
- HRS further reduces environmental impact
- HRS + H_2D results in the best environmental performance
- Reduction of environmental impact by up to 72% by using 'greener' alternatives for electricity and hydrogen production.

For more information see: [Sustainable semiconductor manufacturing: Lessons for lithography and etch | SPIE Advanced Lithography + Patterning]

*Hauglustaine et al, 2022

Imec member of SEMI circularity working group

Being a part of the SEMI circularity working group, imec has **access to a repository of industry best practices** and discusses current **challenges** facing the industry with regards to materials and the **circular economy**.

SEMI Sustainability Initiative

SEMI Standards

As working groups evolve in their deliverables, they will evolve to SEMI Standards Task Forces

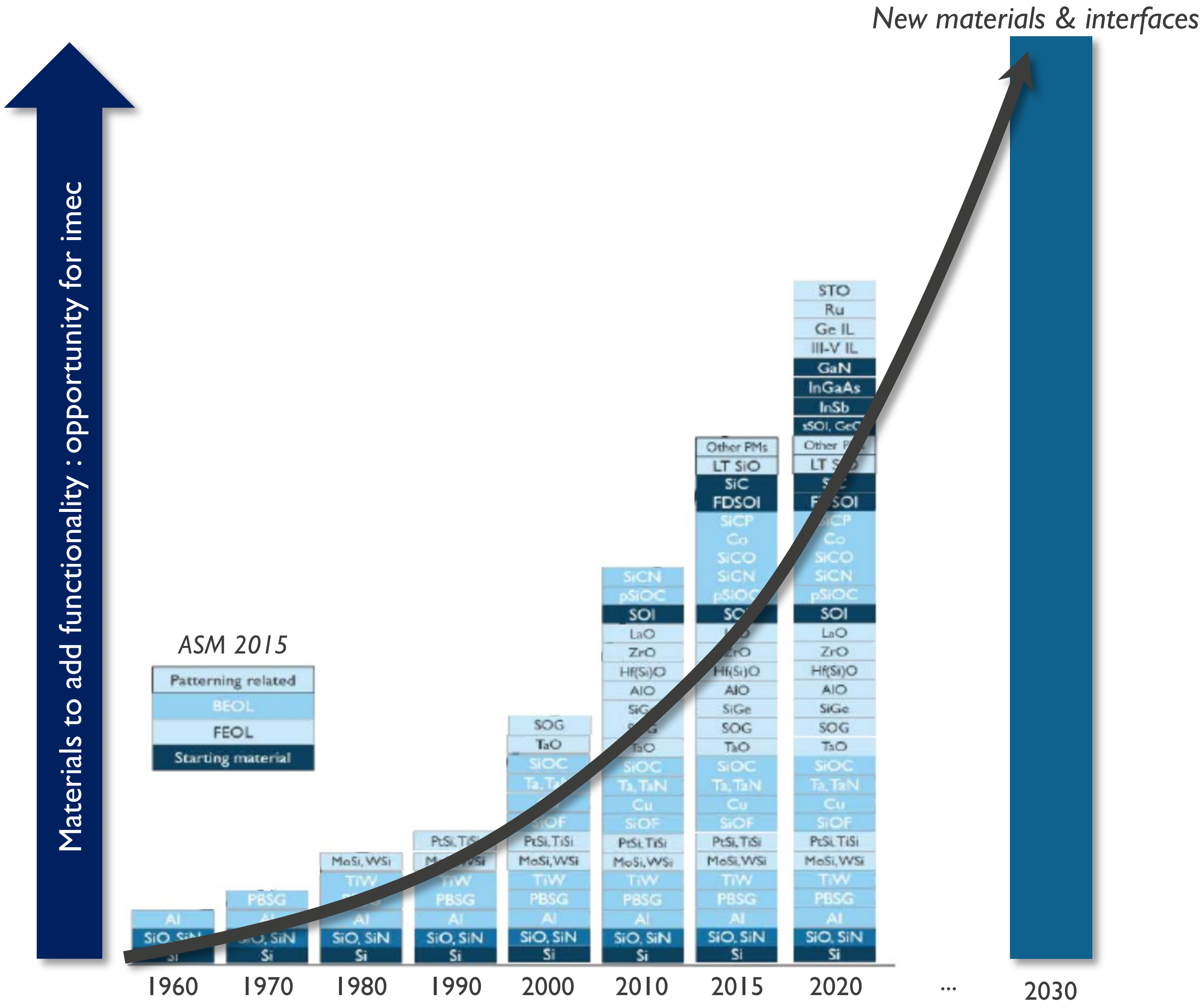
Approach

Benchmark

Innovation through collaboration

Government support

2030 + ?


New materials & interfaces
Materials to add functionality : opportunity for imec
ASM 2015
Patterning related
BEOL
FEOL
Starting material
Si
SiO, SiN
Al
PBSG
TiW
MoSi, WSi
PtSi, TiSi
SiOF
Cu
Ta, TaN
SiOC
TaO
SOG
SiGe
AlO
Hf(Si)O
ZrO
LaO
SOI
pSiOC
SiCN
SiCO
Co
SiCP
FDSOI
SiC
LT SiO
Other PMs
sSOI, GeO
InSb
InGaAs
GaN
III-V IL
Ge IL
Ru
STO
1960
1970
1980
1990
2000
2010
2015
2020
...
2030

imec

embracing a better life