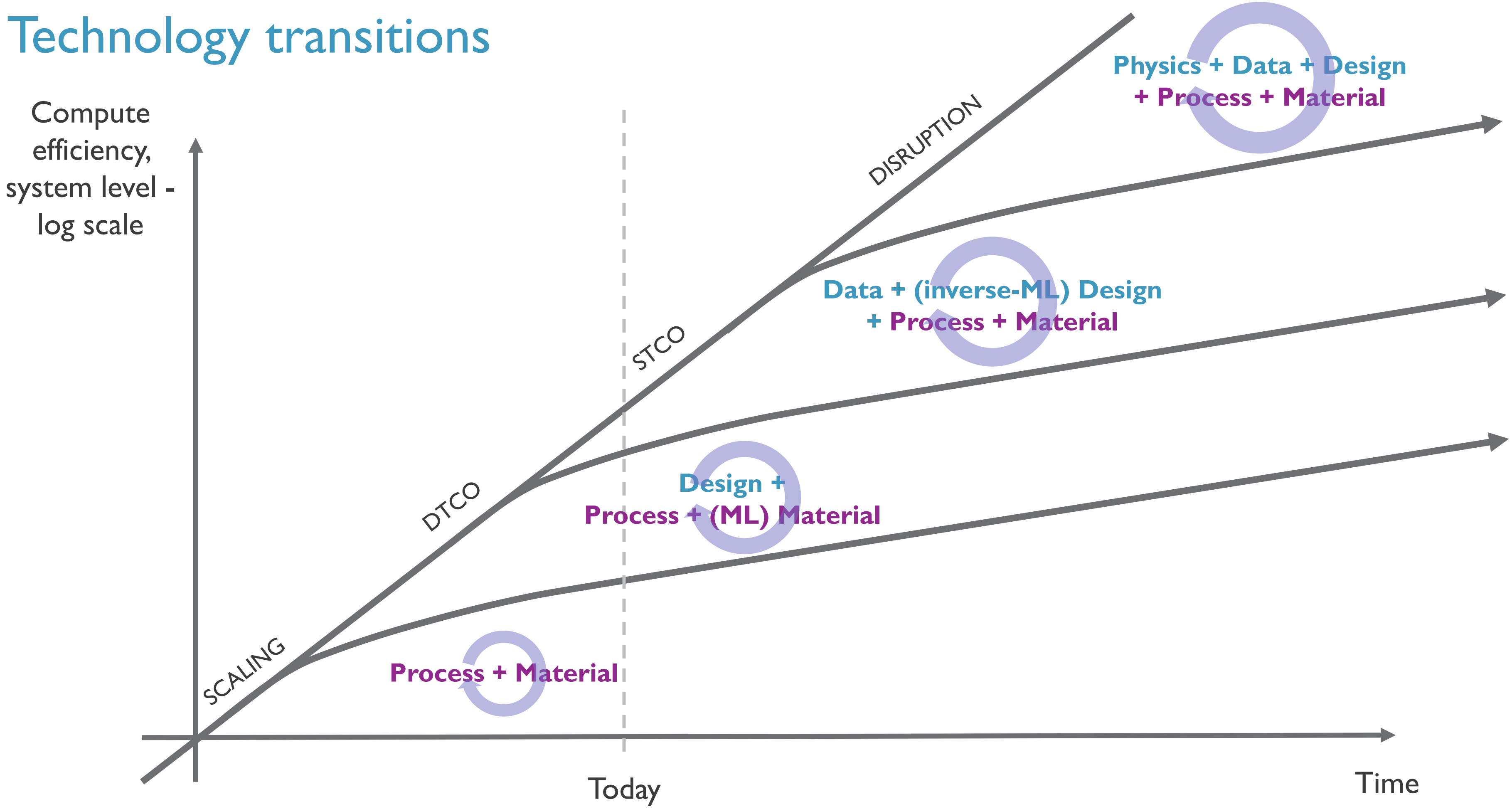
SEMICON
EUROPA

Accelerating nanoelectronic device innovation through atomistic simulation–driven material screening

Geoffrey Pourtois

Technology transitions



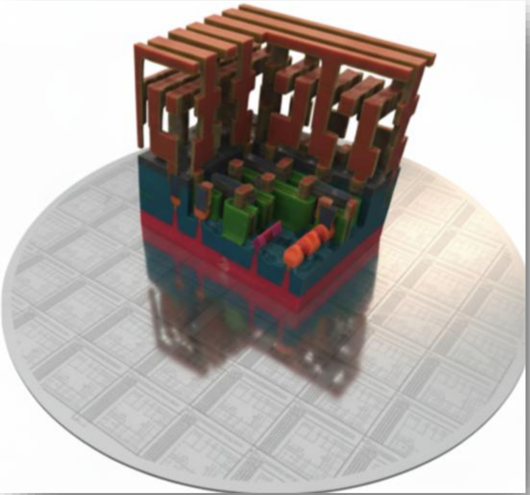
Finding the right materials,...

What do these pictures have in common?

Amorphous SiO_2

Chalcedony spherulites: crypto-crystalline SiO_2

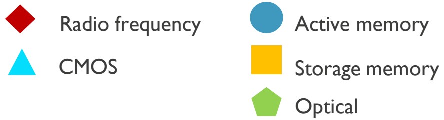
Amorphous SiO_2

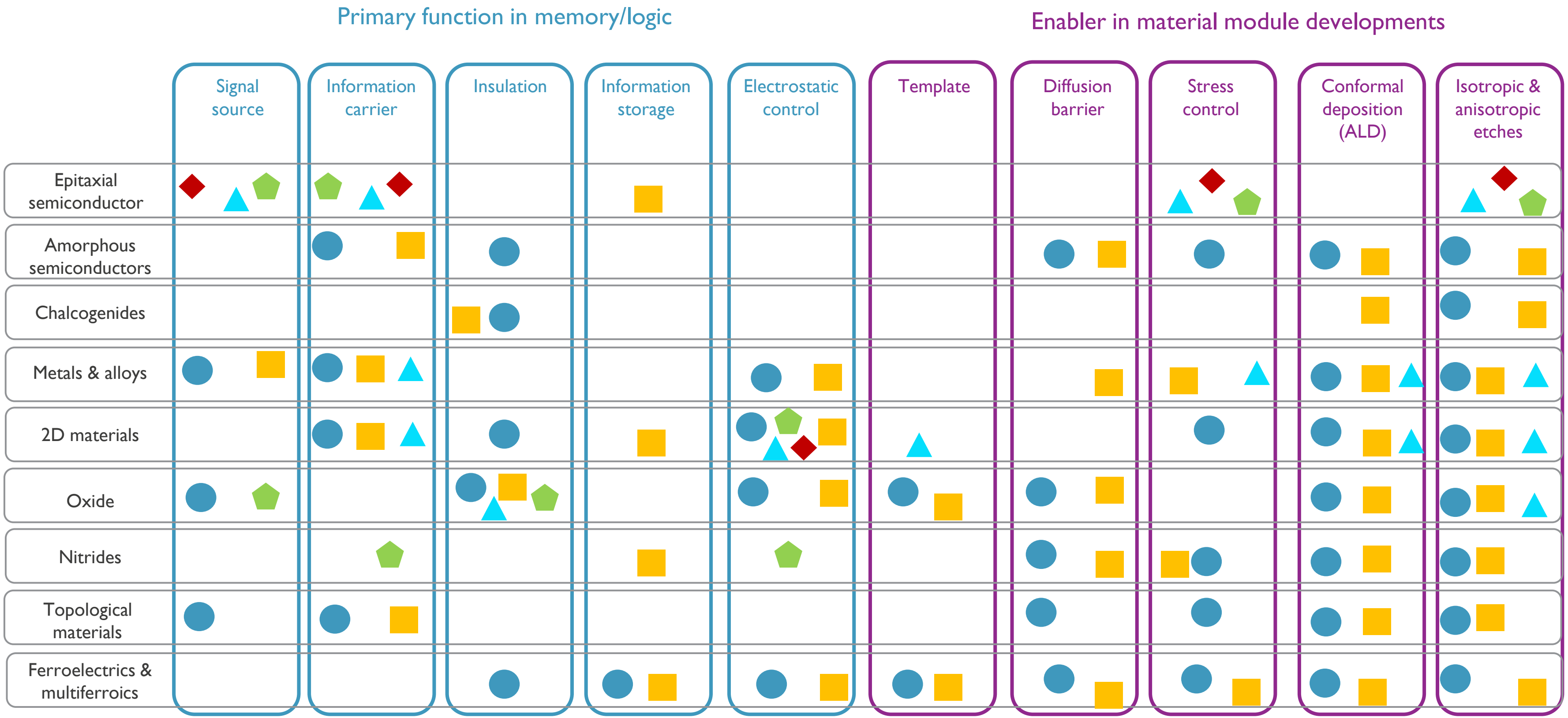


2 nm nanosheet technology

- 1 material = several forms = different functions = different environments

Complex function-application-material matrix



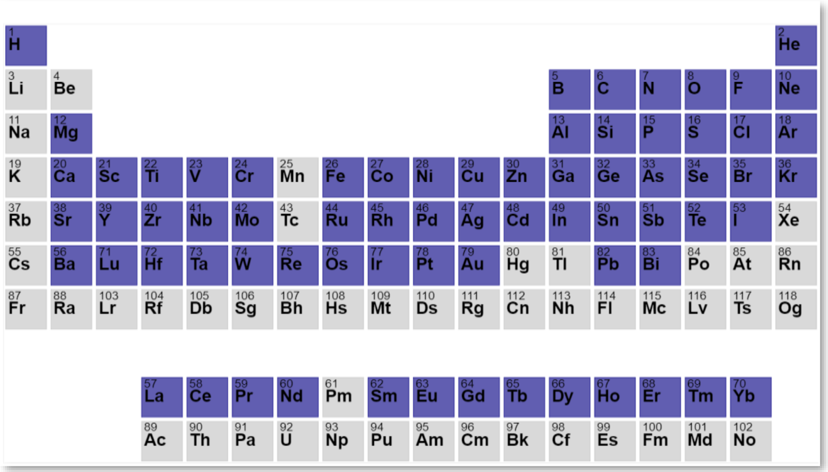


- 1 material = several forms = different functions = different environments

New materials = source of inspiration

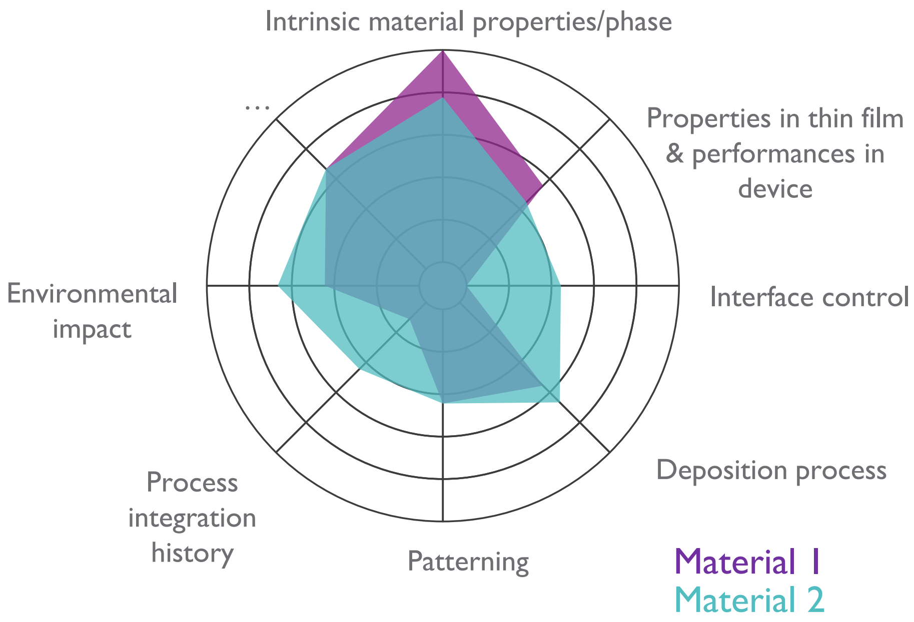
But also of perspiration,...

Elements used in R&D CMOS & memory today



- Chemical space: ~90 dimensions + process & application dependencies

Tackling a N-dimensional problem



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

Material journey: from concept to 300mm pilot line

Multi-level material down-selection process

Literature based data-mining – expected properties

Device Concept → Device specs → Data mining → Material figure of merits → Virtual material screening &/or machine learning → Material exploration in LAB → 300 mm FAB → Evaluation at device scale

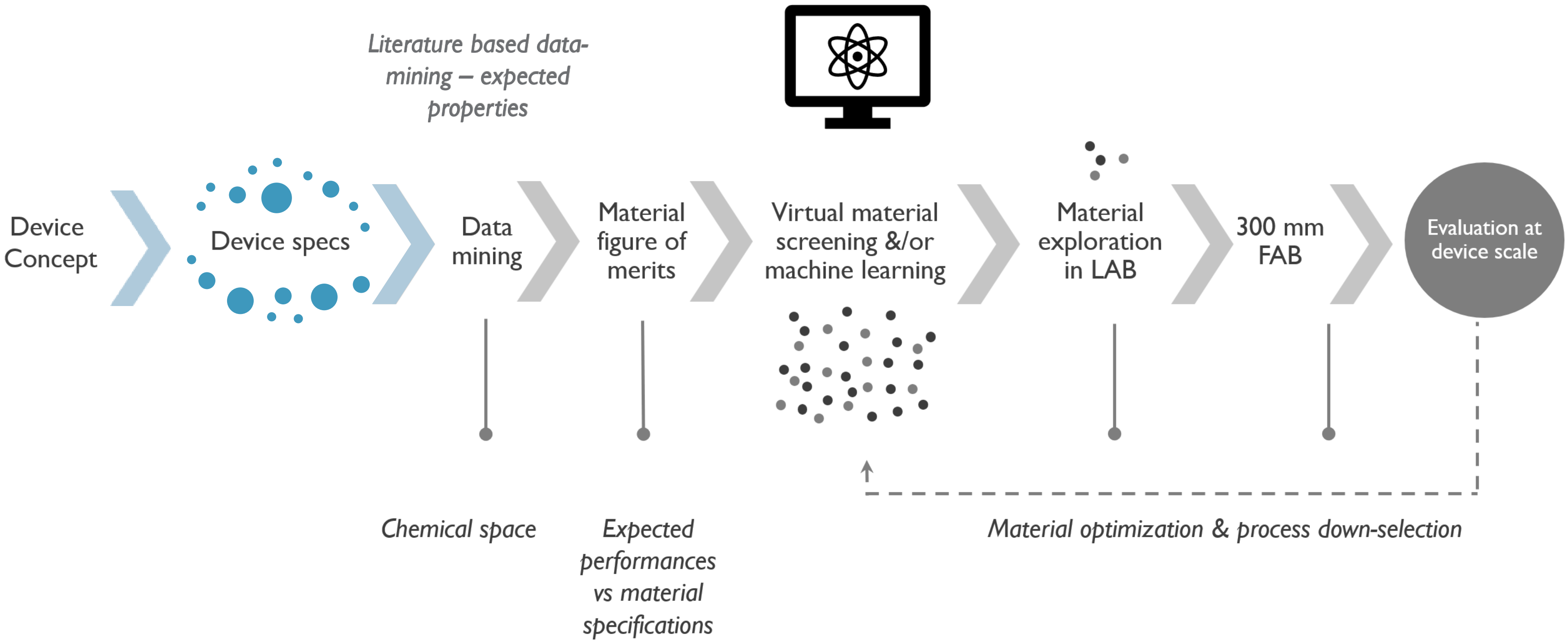
Chemical space

Expected performances vs material specifications

Material optimization & process down-selection

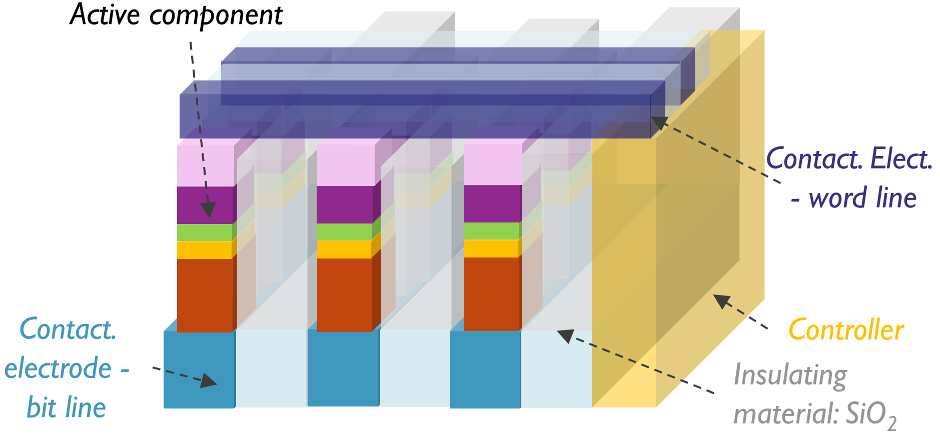
Material journey: from concept to 300mm pilot line

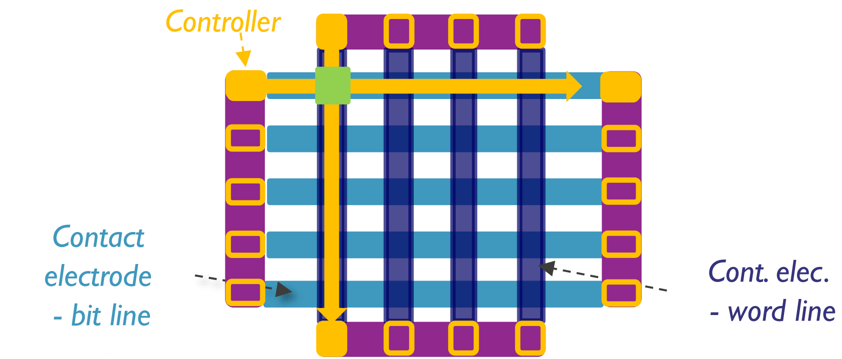
Multi-level material down-selection process



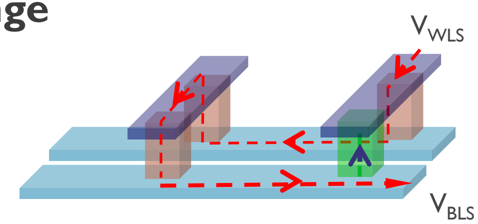
Problem at hand

Addressing a memory bit



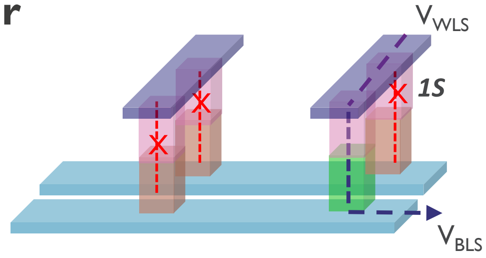


Challenge



- Single memory cell can be mis-read from current sneak-path contributions

Selector

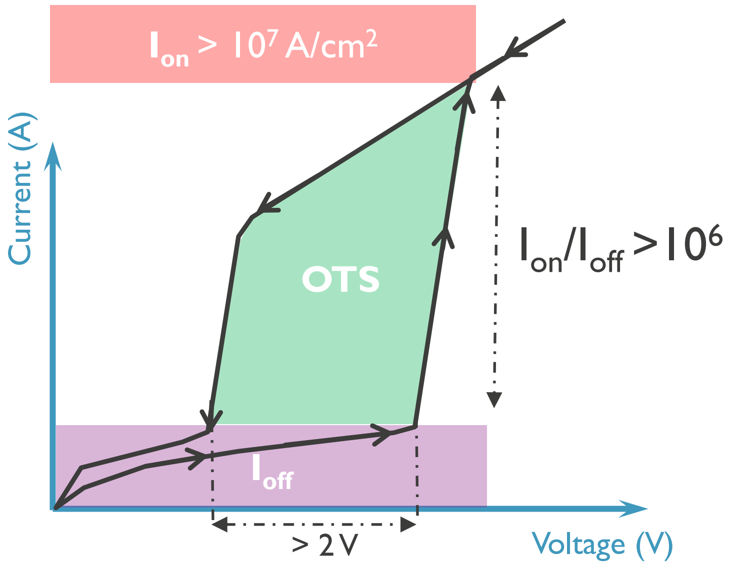


- Materials that mimics some part of a “diode” electrical signature need to be operated as a filtering layer to shut-off sneak leakage current

Requirements

Device specifications for Ovonic Threshold Switch (OTS)[1]

Ideal I.V profile



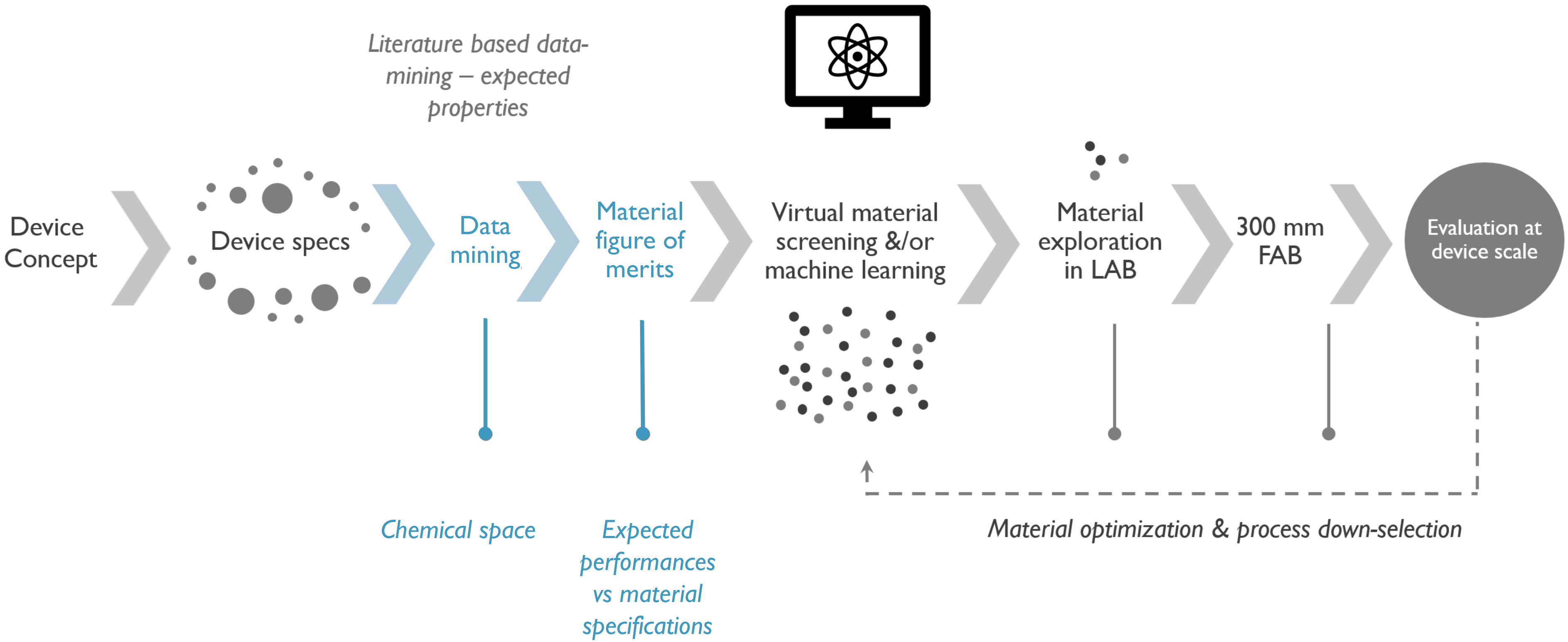
Material requirements

- Semiconductor (amorphous)
- Mobility gap ≥ 1.5 eV
- Low density of defects (10^{19}cm^{-3})
- $T_{cryst}/T_{melting}$ ≥ 400 °C
- Low T deposition, conformality
- Material thickness min: 4 nm
- High non-linear signature
- No phase transition

- Need “smart” data driven choices of “context aware” materials

Material journey: from concept to 300mm pilot line

Multi-level material down-selection process



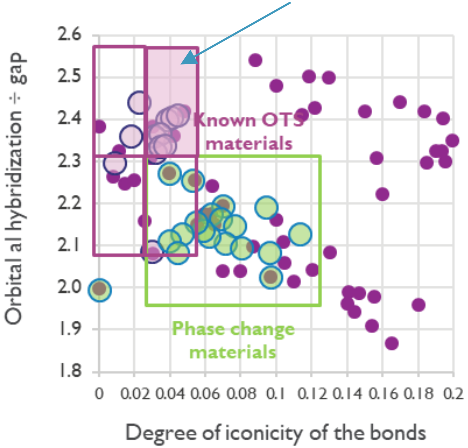
Material journey: from concept to 300mm pilot line

Multi-level material down-selection process

"PCM-like" family

- $> 10^6$ possible combinations
- No phase change allowed

Data mining

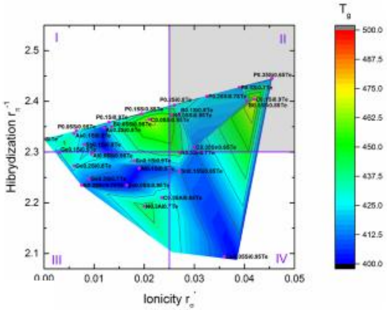


- Semi-empirical model that links material orbitals and bond ionicity with phase change character

+

Phase transition

Ex: Te ternary alloys



- Glass transition temperature needs to be as high as possible [1]

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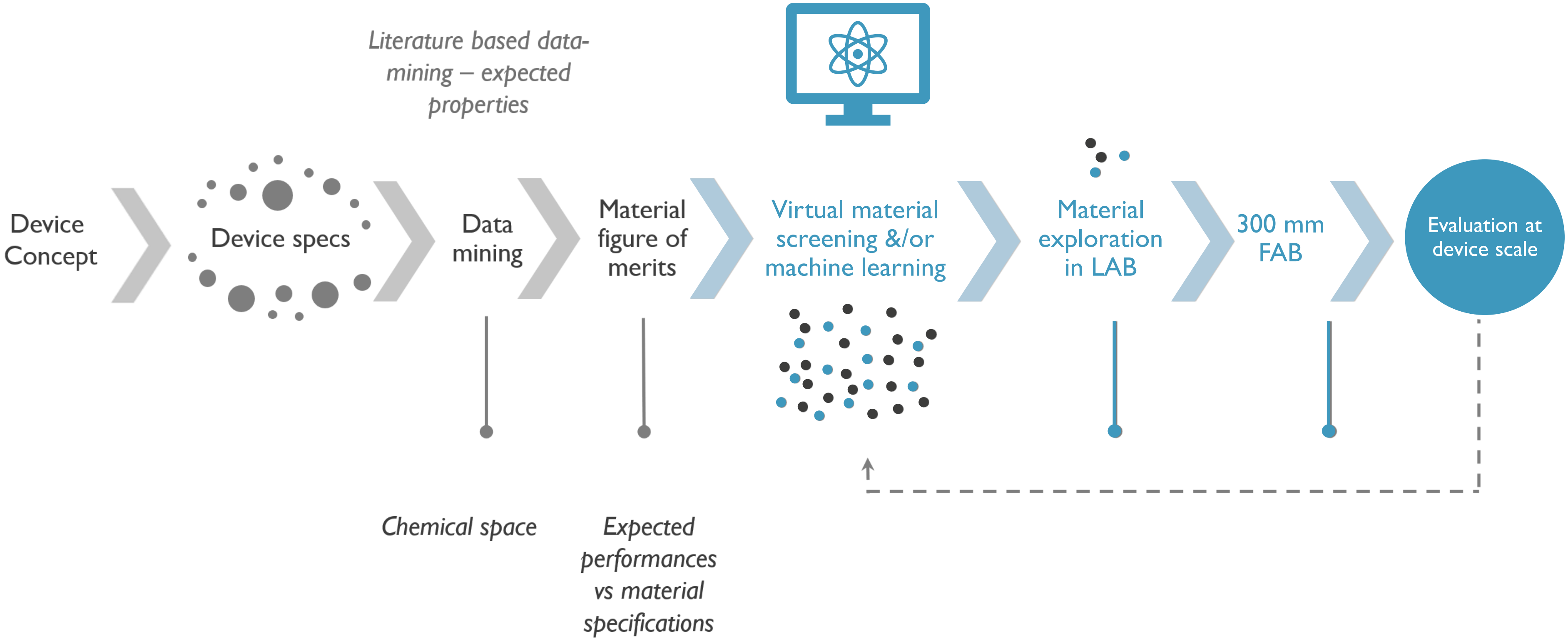
Element down-selection

- Ge based alloys with $>10^4$ possible combinations

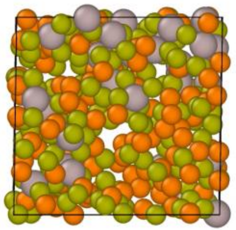
Material journey: from concept to 300mm pilot line

Multi-level material down-selection process

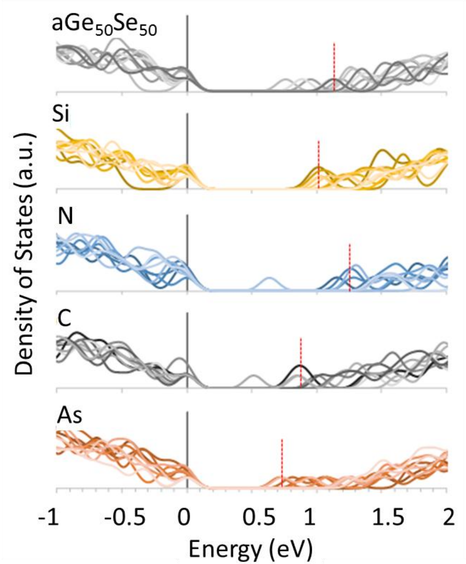


Material screening

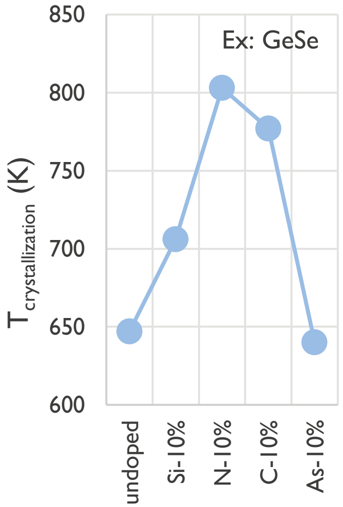
Atomistic simulations



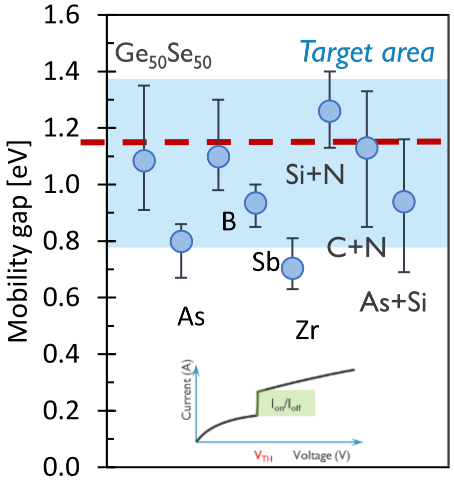
Electronic properties



Crystallization T



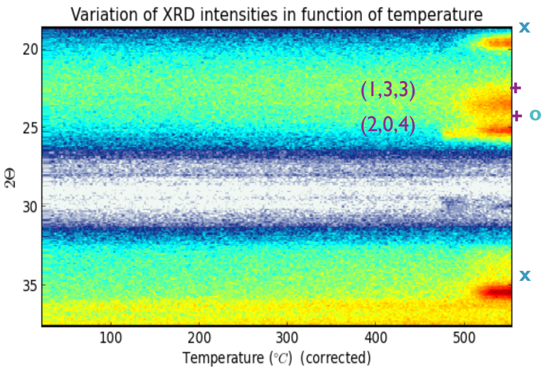
Band gap



- Selected alloys from the screening include elements such as Si, Ge, As, and Te/Se
- Se based alloys: T_{crys} is too low → engineering through doping is required
- Doping = band gap and defect level modulations
- Modulation of I_{on}/I_{off}

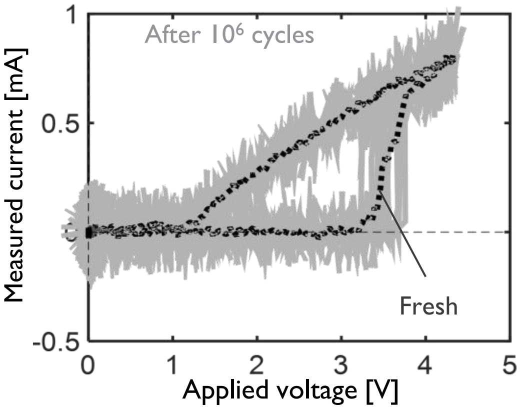
Further funneling

@LAB level



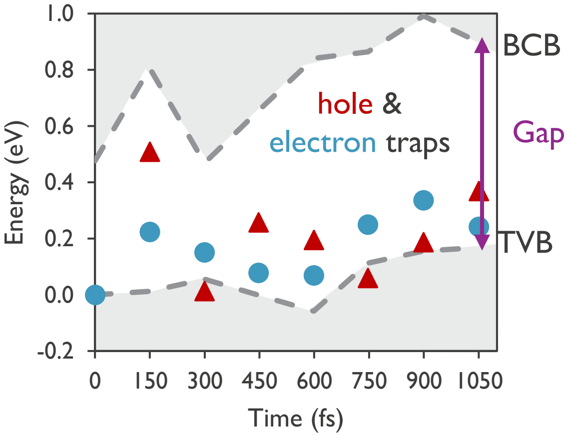
- Quantification of phase transition T
- Thermal & electrical performances
- Element selection: Si,Ge,As,Te/Se

Device performances



- Drift of electrical signature, V_{th} shift → problematic

Dynamic evolution of the electronic properties[1]

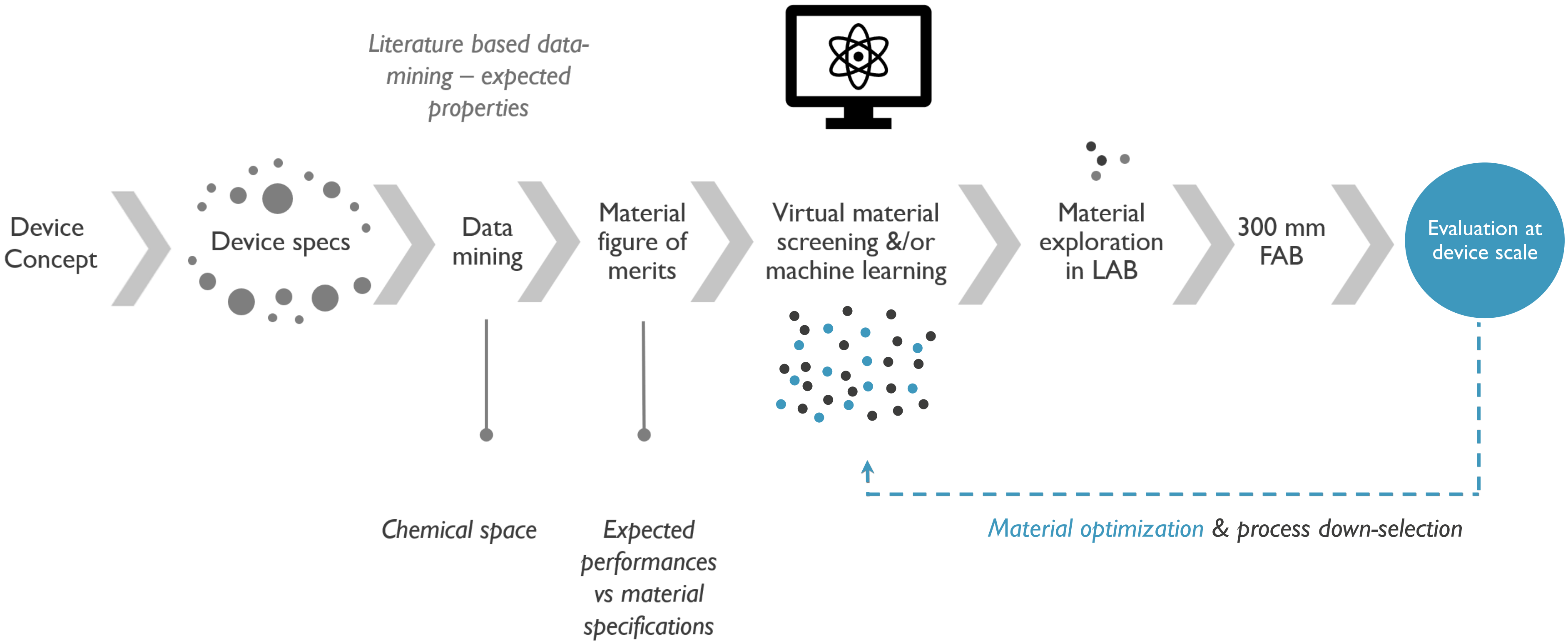


- Alloys contain poisonous elements: As,Te → not an ideal solution
- Drift of electronic properties

- Going back to the drawing board is needed

Material journey: from concept to 300mm pilot line

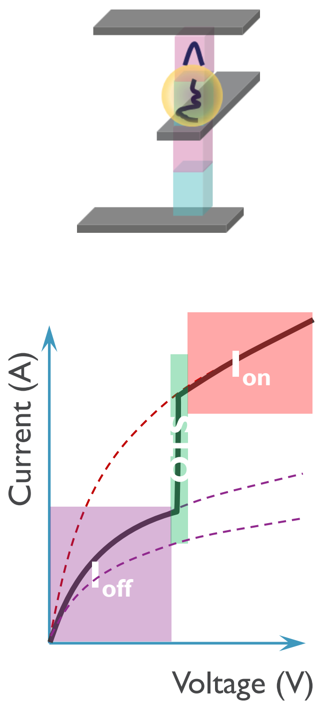
Multi-level material down-selection process



[1] S. Clima et al, npj Computational Materials 9 (1), 96 (2023)

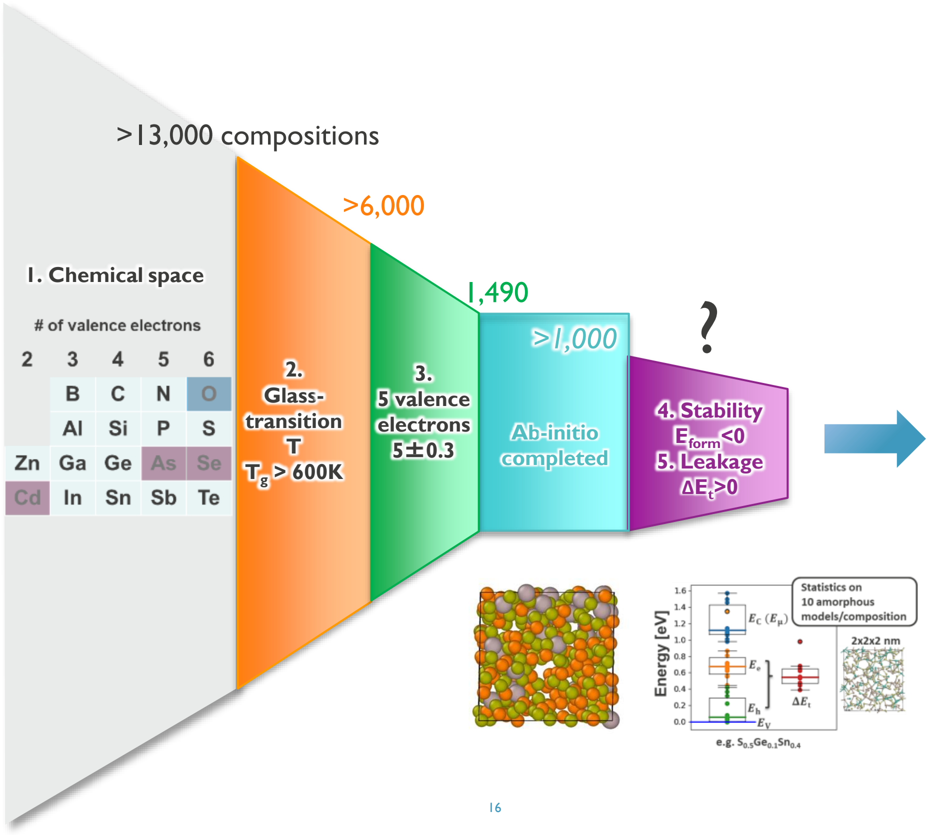
Identification of As/Se-free OTS materials[1]

Ideal I.V profile



Chemical space

Virtual material screening

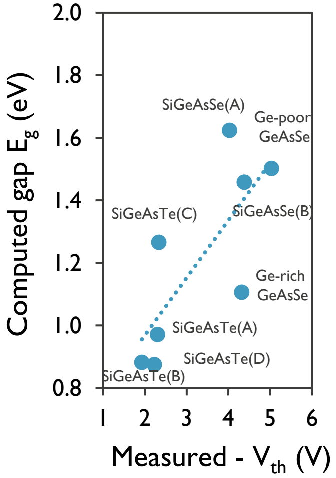


Evaluation of material stability and anticipated electrical performances

[1] Clima et al., ACS Applied Electronic Materials 5 (1), 461-469 (2023)
[2] S. Clima et al, IEDM (2024), D. Matsubayashi et al, IEDM (2022)

Linking material properties to electrical performances

Correlations [1,2]



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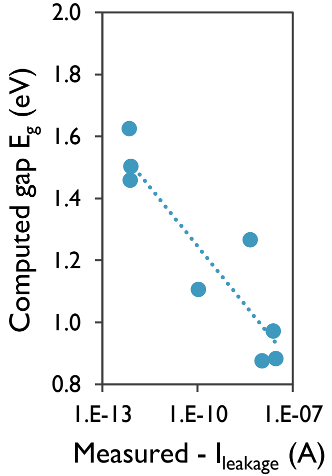

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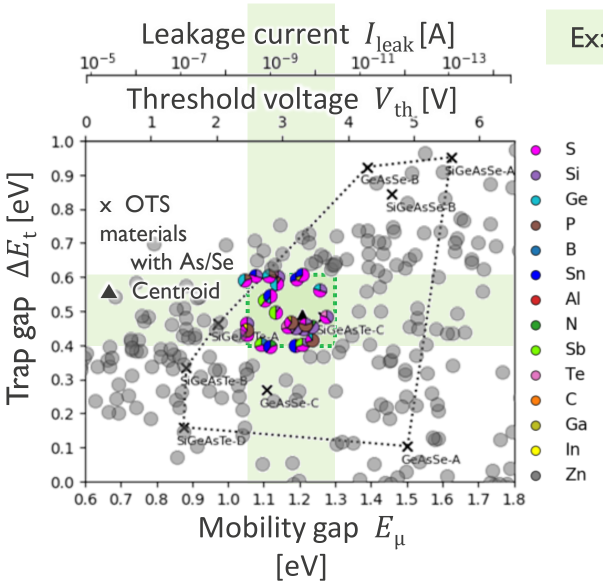
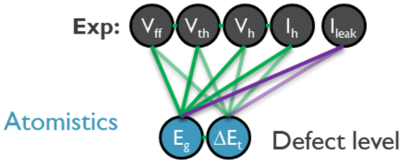
Mapping electrical performances to materials [1,2]

Ex: RRAM selector



New material candidates

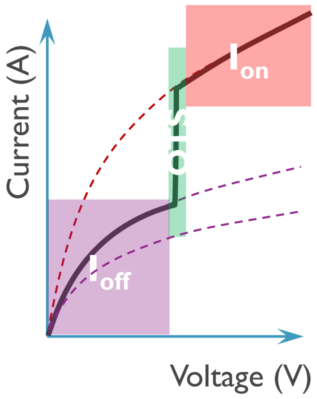
Identified correlations:



[1] Clima et al., ACS Applied Electronic Materials 5 (1), 461-469 (2023)
[2] S. Clima et al, IEDM (2024), D. Matsubayashi et al, IEDM (2022)
[3] US 2024/0188456 A1 ; US 2024/0188457 A1[1]; EP 4380334 B1

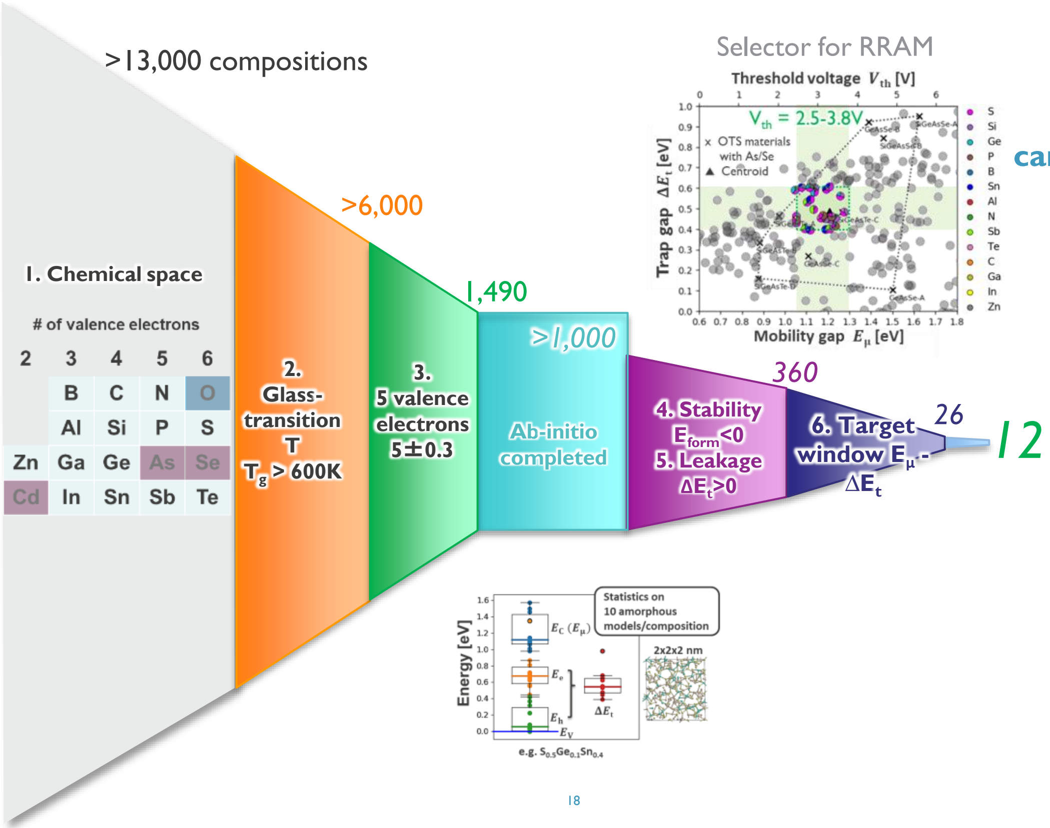
Identification of As/Se-free OTS materials

Profile



Chemical space

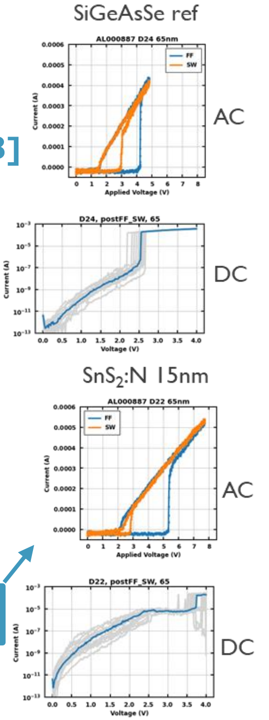
Virtual material screening



Electrical tests

12 identified candidates[1,2,3]

- P0.2S0.4Ge0.4
- Si0.3S0.5Sn0.2
- Si0.3S0.5Ge0.2
- S0.5Ge0.1Sn0.4
- Si0.4S0.3Te0.3
- P0.1S0.4Ge0.5
- Si0.2S0.5Sn0.3
- Si0.4S0.4Te0.2
- Si0.5S0.4Te0.1
- P0.3S0.4Ge0.3
- Si0.4P0.3S0.3
- N0.1S0.6Sn0.3



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Device Concept

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Material figure of merits

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Material exploration in LAB

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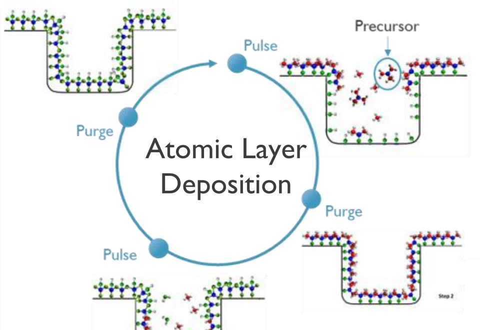
Expected performances vs material specifications



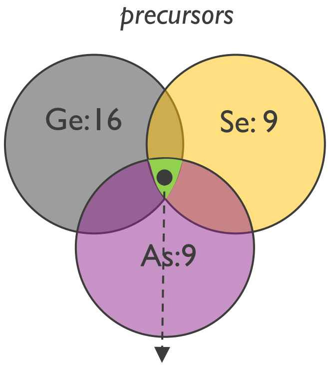
V. Cremers et al., Appl. Phys. Rev., 2019, 6, 021302

[1] B. van der Linden et al, J. Phys. Chem. C, vol. 129 pp 19573 (2025)
[2] Courtesy of Tobias Peissker

Precursor selection for conformal deposition

Ex: GeSeAs

Process for conformal deposition (ALD)



ALD process independent of the sequence order

- 1000+ precursors and injection sequence combinations

Computed enthalpy of reactions

Ge-As

	$As(NMe_2)_3$	$AsEt_3$	AsH_2Et	$AsH_2(^tBu)$	AsH_3	$As(SiEt_3)_3$	$AsCl_3$	$As(OEt)_3$	$As(OMe)_3$
$GeEt_4$	-0.02	-0.66	-0.83	-0.77	-0.93	-0.25	0.17	0.05	0.04
GeH^nBu_3	-0.08	-0.66	-0.32	-0.22	-0.39	-0.19	0.21	0.10	0.09
GeH_2Et_2	-0.10	-0.67	-0.31	-0.27	-0.35	-0.23	0.25	0.11	0.10
GeH_2Me_2	0.03	-0.56	-0.30	-0.24	-0.33	-0.26	0.47	0.34	0.34
GeH_4	-0.45	-0.91	-0.27	-0.23	-0.29	-0.29	-0.01	-0.35	-0.35
H_2GeCl_2	1.61	0.33	0.29	0.15	0.09	-0.51	2.39	2.51	2.55
$HGeCl_3$	1.44	0.15	0.18	0.03	-0.02	-0.58	2.31	2.39	2.44
$GeH(SiEt_3)_3$	-0.21	-0.50	-0.22	-0.07	-0.37	0.65	-0.17	-0.51	-0.53
$Ge(SiEt_3)_4$	-0.65	-0.68	-0.61	-0.46	-0.76	0.73	-1.41	-1.47	-1.50
$Ge(O^nBu)_4$	1.37	-0.01	-0.04	-0.13	-0.41	-1.05	2.53	2.71	2.72
$Ge(OEt)_4$	1.34	-0.02	-0.05	-0.14	-0.42	-1.06	2.53	2.70	2.71
$Ge(OMe)_4$	1.30	-0.06	-0.08	-0.18	-0.44	-1.11	2.55	2.68	2.68
$Ge(NMe_2)_4$	1.11	-0.32	-0.39	-0.29	-0.65	-0.44	1.46	1.31	1.32
$Ge(N(SiMe_3)_2)_2$	0.75	0.22	0.09	0.62	-0.54	-0.31	1.58	1.78	1.79
$GeCl_4$	1.00	-0.15	-0.02	-0.16	-0.22	-1.18	2.20	2.20	2.26
$GeCl_2$	1.37	0.91	0.78	0.64	0.58	-0.55	2.55	2.52	2.59

∩

Ge-Se

	$Se(OMe)_2$	$Se(NMe_2)_2$	$SeCl_2$	$SeEt_2$	H_2Se	$Se(Si^iPr_3)_2$	$Se(SiEt_3)_2$	$Se(SiMe_3)_2$	$Se(SnMe_3)_2$
$GeEt_4$	-0.82	-1.06	-0.91	-1.02	-1.13	-0.11	-0.13	-0.18	0.27
GeH^nBu_3	-0.71	-0.96	-0.80	-0.96	-0.58	-0.09	-0.03	-0.06	0.23
GeH_2Et_2	-0.69	-0.93	-0.72	-0.90	-0.50	-0.10	-0.11	-0.08	0.33
GeH_2Me_2	-0.45	-0.81	-0.51	-0.80	-0.48	-0.19	-0.07	-0.05	0.32
GeH_4	-1.04	-1.29	-1.00	-1.11	-0.36	-0.08	0.03	0.07	0.33
H_2GeCl_2	1.71	0.81	1.40	0.10	-0.00	-0.21	-0.09	-0.07	0.13
$HGeCl_3$	1.72	0.78	1.43	0.01	-0.04	-0.20	-0.08	-0.06	0.14
$GeH(SiEt_3)_3$	-1.35	-1.41	-1.28	-0.80	-0.50	0.57	0.51	0.42	0.45
$Ge(SiEt_3)_4$	-2.32	-1.84	-2.52	-1.08	-0.89	0.51	0.41	0.26	0.14
$Ge(O^nBu)_4$	1.78	0.64	1.41	-0.18	-0.48	-0.74	-0.60	-0.64	0.27
$Ge(OEt)_4$	1.77	0.62	1.41	-0.18	-0.49	-0.75	-0.60	-0.70	0.28
$Ge(OMe)_4$	1.75	0.60	1.43	-0.21	-0.51	-0.78	-0.71	-0.73	0.19
$Ge(NMe_2)_4$	0.47	0.13	0.29	-0.60	-0.83	-0.35	-0.32	-0.36	0.42
$Ge(N(SiMe_3)_2)_2$	0.66	0.01	0.29	-0.57	-1.12	-0.14	-0.46	-0.50	0.05
$GeCl_4$	1.55	0.59	1.30	-0.10	-0.13	-0.78	-0.69	-0.64	-0.44
$GeCl_2$	1.69	0.40	1.25	0.10	-0.04	[redacted]	[redacted]	[redacted]	[redacted]

∩ ∩

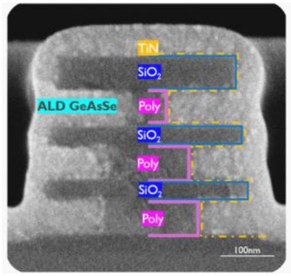
As-Se

	$Se(OMe)_2$	$Se(NMe_2)_2$	$SeCl_2$	$SeEt_2$	H_2Se	$Se(Si^iPr_3)_2$	$Se(SiEt_3)_2$	$Se(SiMe_3)_2$	$Se(SnMe_3)_2$
$AsEt_3$	-0.89	-1.06	-0.87	-1.01	-1.05	-0.20	-0.20	-0.22	0.23
AsH_2Et	-0.76	-0.93	-0.70	-0.87	-0.32	-0.06	0.07	0.10	0.42
$AsH_2(^tBu)$	-0.86	-0.83	-0.84	-0.86	-0.33	0.30	0.18	0.10	0.54
AsH_3	-1.12	-1.19	-0.90	-0.98	-0.20	0.06	0.19	0.23	0.50
$As(SiEt_3)_3$	[redacted]	[redacted]	[redacted]	[redacted]	-0.21	0.77	0.70	0.65	0.56
$As(OEt)_3$	1.60	0.45	1.21	-0.29	-0.59	-0.88	-0.80	-0.77	0.18
$As(OMe)_3$	1.60	0.45	1.24	-0.31	-0.59	-0.89	-0.81	-0.79	0.17
$As(NMe_2)_3$	0.34	-0.03	0.08	-0.70	-0.90	-0.56	-0.53	-0.53	0.29
$AsCl_3$	1.48	0.49	1.15	-0.08	-0.14	-0.79	-0.68	-0.62	-0.40

Precursor selection

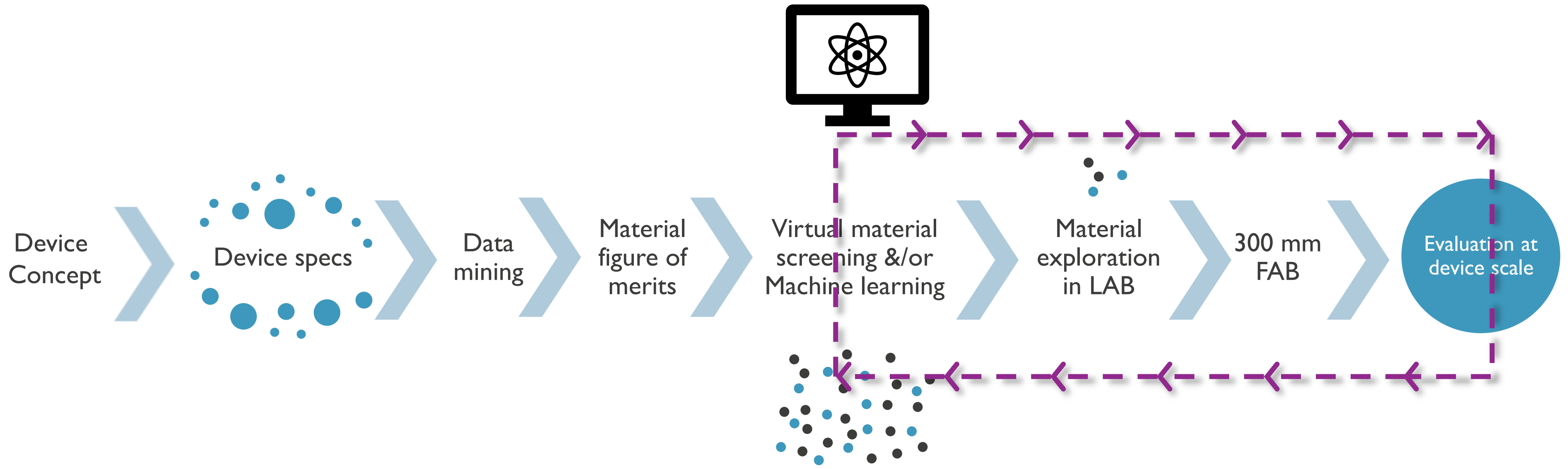
- Ex: $C_4H_6O_2.GeCl_2$ + H_2Se + $As(SiEt_3)_3$
- Other combinations have been identified

Achieved conformal deposition [2]



Material journey: from concept to 300mm pilot line = multi-dimensional problem

Multi-level material down-selection process



Thank you to,…

The best modeling and ALD teams ever (in imec)

Modeling

Sergiu Clima

Kiroubanand Sankaran

Michiel van Setten

Benoit Van Troeye

Christopher Pashartis

Laura Galleni

Bram van der Linden

Ula Kocur

Zifei Shen

Material deposition

Tobias Peissker

Sebastiaan Nijs

And to the "active memory" research program of imec, imec colleagues and IIAP core partners.

Thank you for your attention

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