First-principles calculations as a backbone for the development of semiconductor technologies

10th Abinit International Developer Workshop 2021

Benoit Van Troeye, Geoffrey Pourtois

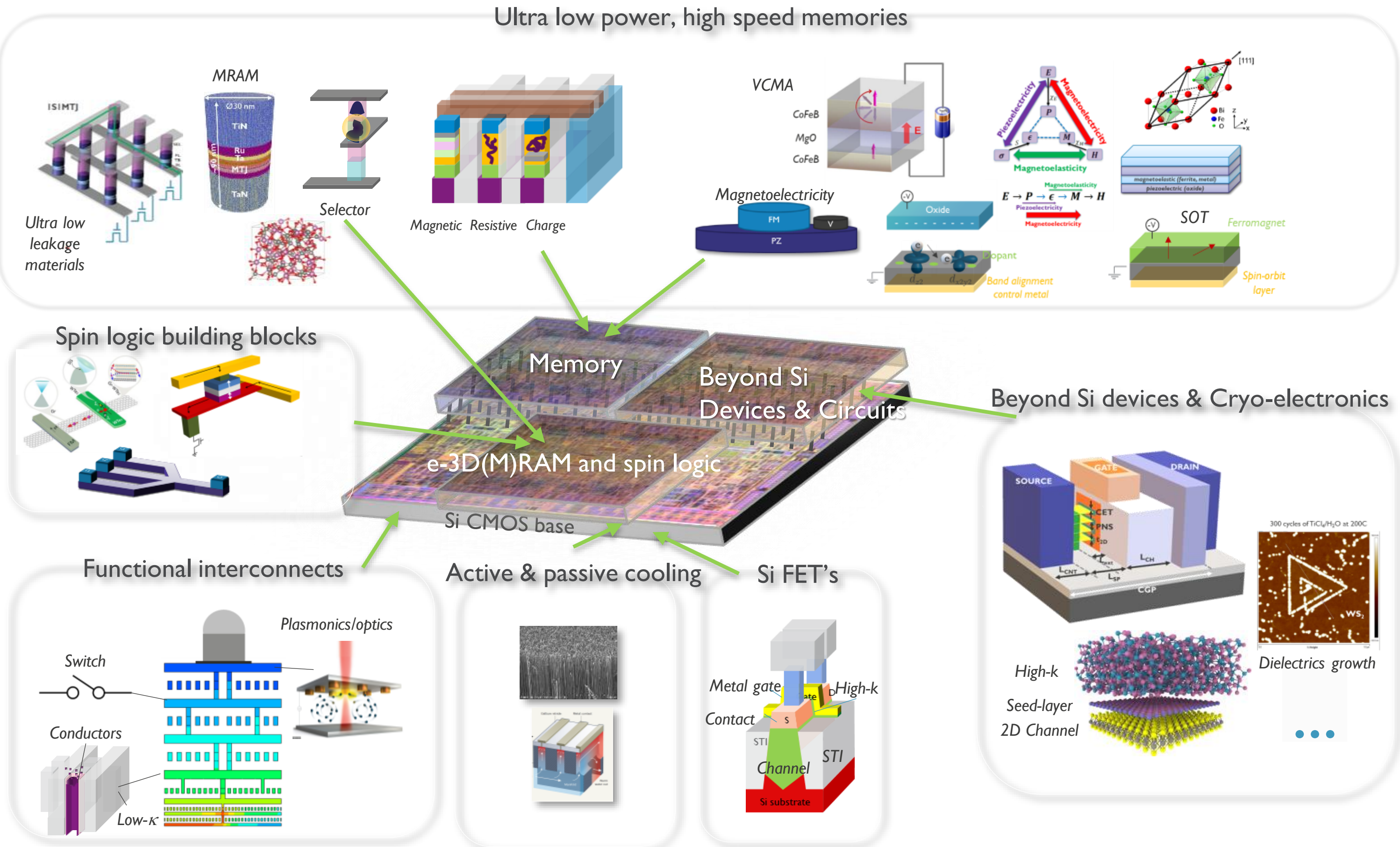
What is IMEC ?

Site at Leuven

R&D hub for nano-and digital technologies
(>4500 employees)

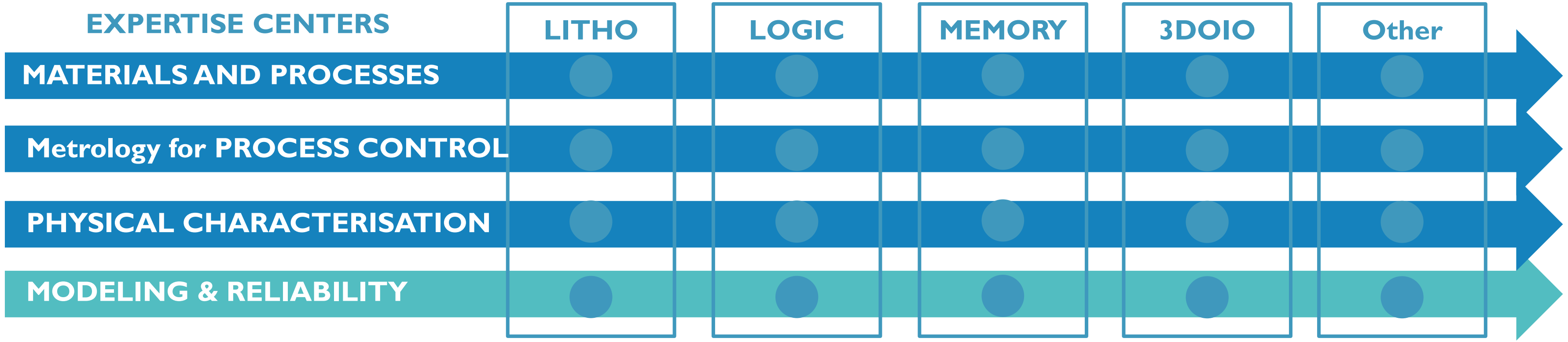
public

2030 + ?



Ultra low power, high speed memories
MRAM
Selector
Ultra low leakage materials
Magnetic Resistive Charge
VCMA
CoFeB
MgO
CoFeB
Magnetoelectricity
FM
PZ
Oxide
Dopant
Band alignment control metal
Magnetoelasticity
SOT
Ferromagnet
Spin-orbit layer
Spin logic building blocks
Memory
Beyond Si Devices & Circuits
e-3D(M)RAM and spin logic
Si CMOS base
Beyond Si devices & Cryo-electronics
SOURCE
GATE
DRAIN
High-k
Seed-layer
2D Channel
Dielectrics growth
• • •
Functional interconnects
Switch
Plasmonics/optics
Conductors
Low-κ
Active & passive cooling
Si FET's
Metal gate
High-k
Contact
STI
Channel
Si substrate

Core CMOS & Memory expertise centers



ATOMISTIC MODELING ACTIVITIES WITHIN IMEC

Optical-Proximity Correction

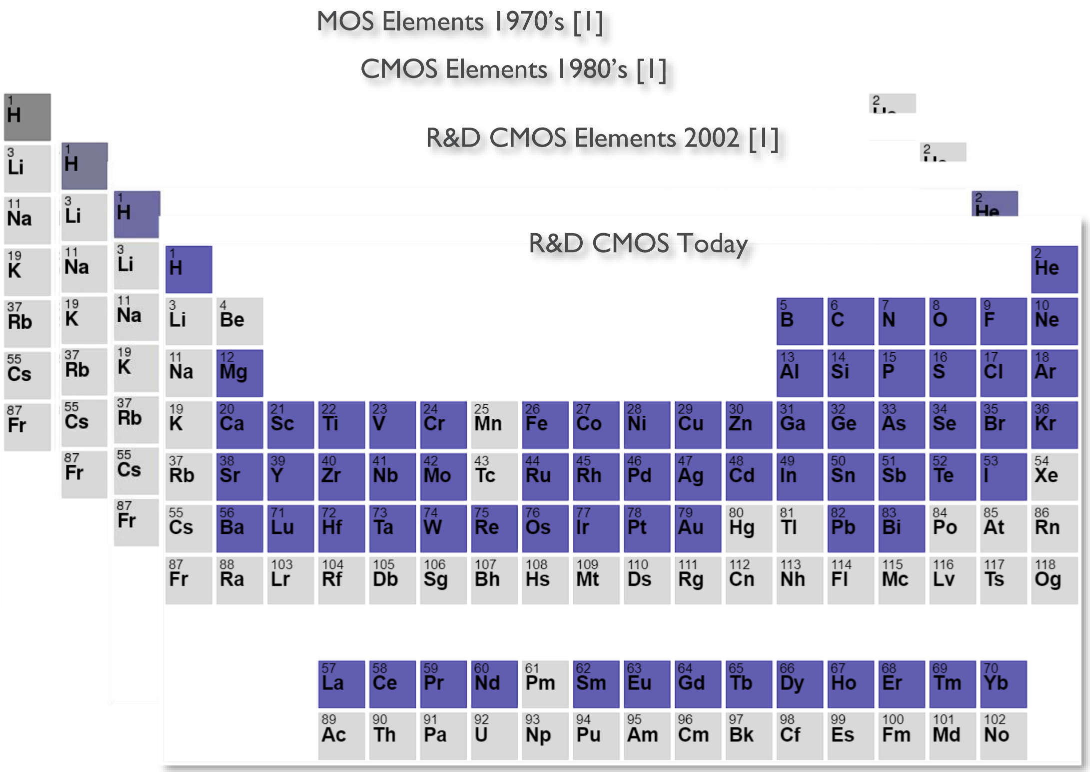
Compact & circuit modeling, TCAD, ***mechanical, thermal and electrical*** *reliabilities, physical, exploratory devices,* ***atomistic modeling,…***

Optical, thermal, mechanical, reliability,…

Acoustics, optical, TCAD, fluidics,…

New materials = source of inspiration

but also of perspiration, ...

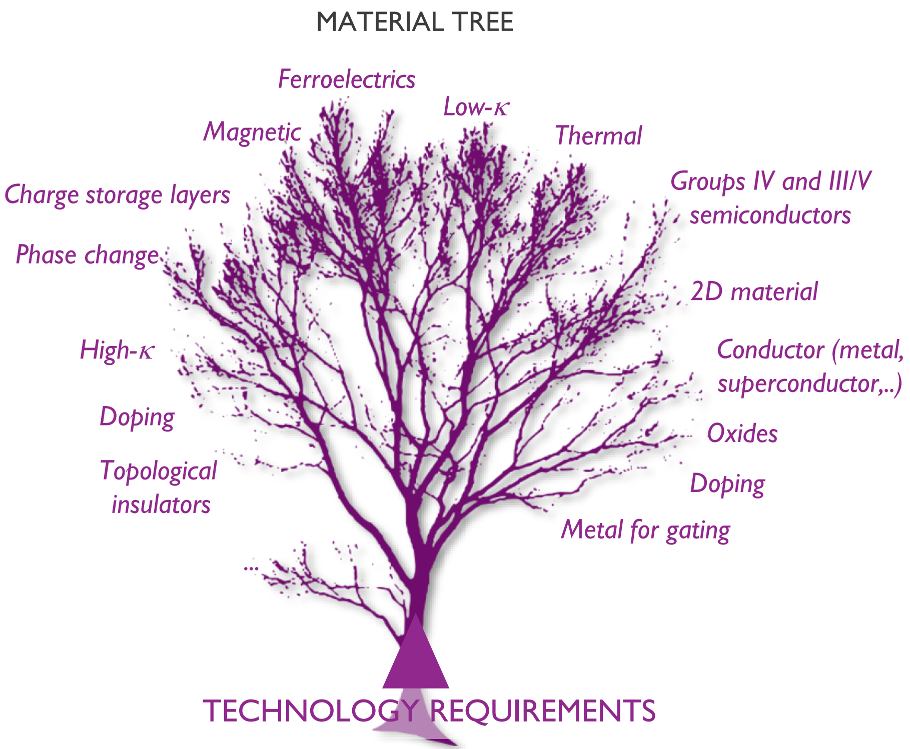


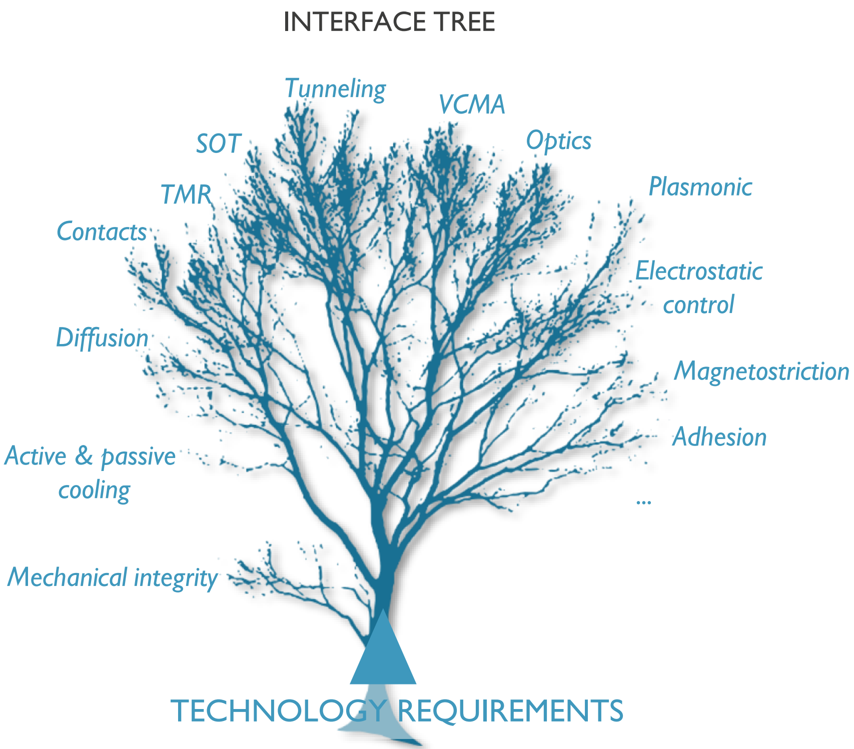
Large number of possible combinations

One material = different functions & phases

Selection process ?

MATERIAL AND TECHNOLOGY





Challenges:

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

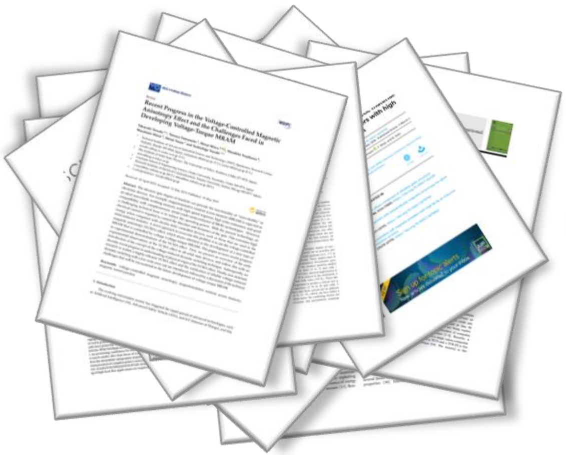
Material journey: from concept to 300mm angstrom Material pilot line

Lab

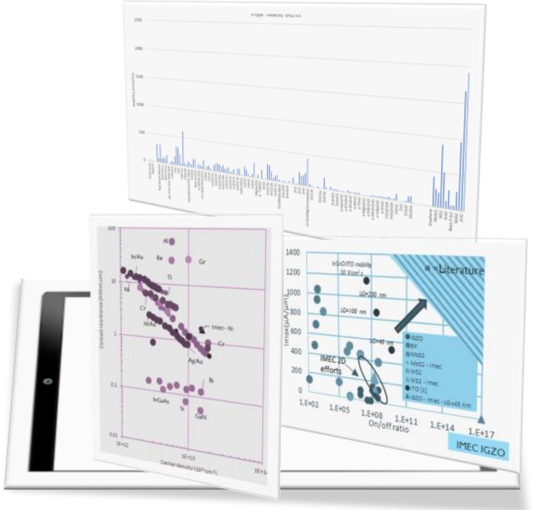
Virtual & proof of concept

- 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

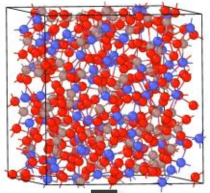
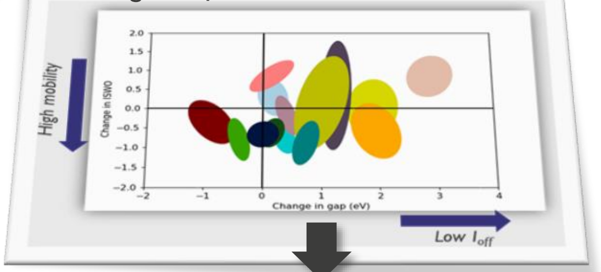


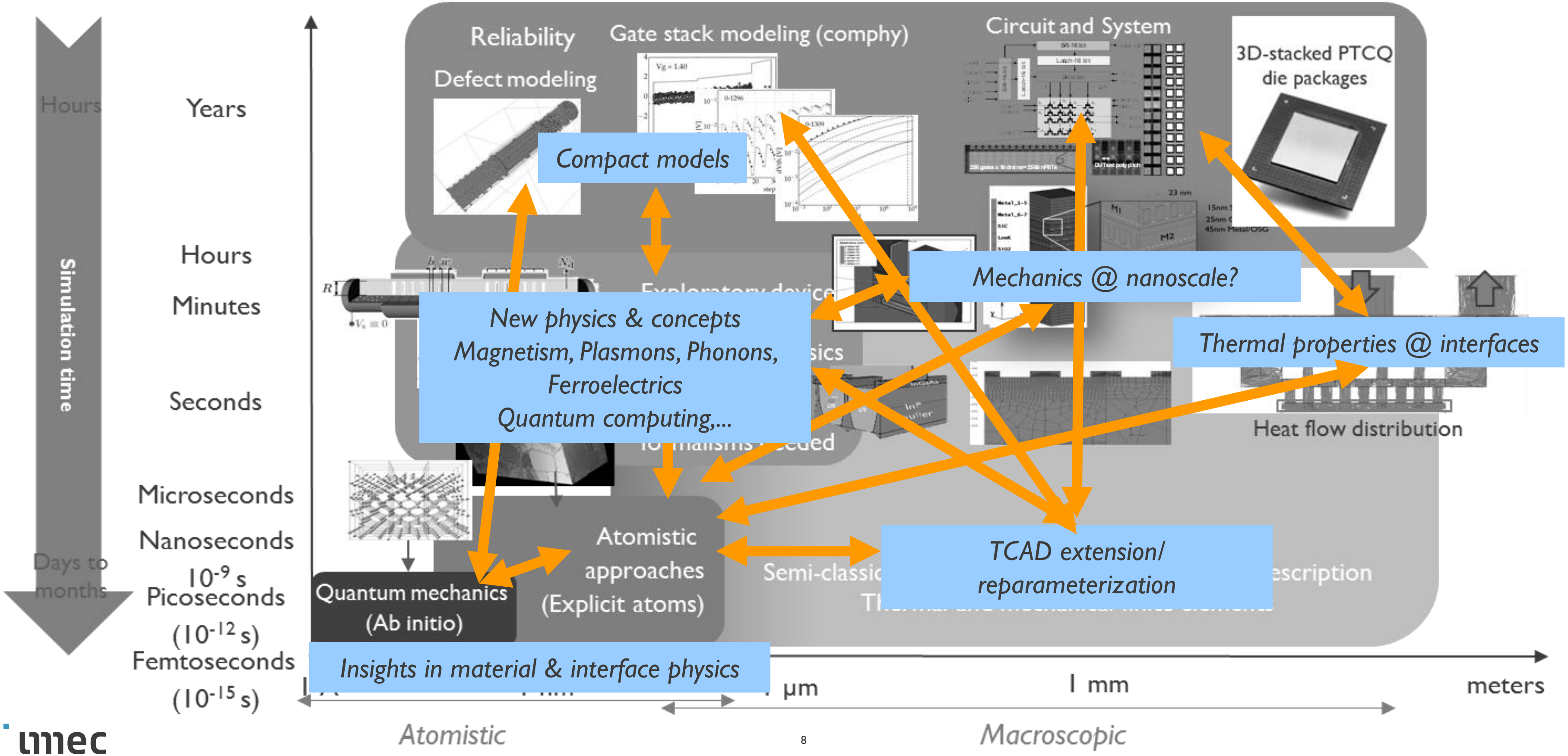
Figure of merits & material selection



LAB/FAB

Modeling playground

Building bridges between modeling approaches



imec
public

Material screening & multiscale effort

Ab initio
Quantum mechanics

Ad-hoc solution: imec in house workflows

Ab initio

Material screening
- Material crystal databases & amorphous generation techniques
- Phase diagram & solubility
- Development of specific properties: meff, gap, magnetic properties, statistics, defects, el. properties, thermal properties

Gate stack & surface chemistry
- Thermodynamics
- Phonons and their derivatives
- Thermodynamic database

Thermal related
- Material crystal structures
- Dielectric properties
- Phonons and their derivatives
- Boltzmann transport solver
  2D monte Carlo Solver
- Temp. prof., spectral flux in devices
  Callibr. & benchmark with exp.

Mechanical
- Material structures
- Mechanical properties of thin films, interface properties
- Finite Element Modeling
- Mechanical properties @ device level

Electrical
- Material Interf./devices
- Electronic structure, Hamiltonian
- NEGF
- Device performances

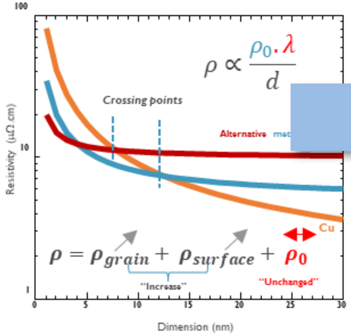
Spectroscopy
- Molecule, material crystal or amorphous
- Excited states & spectroscopy
- Material database to design of photoresists

Under development

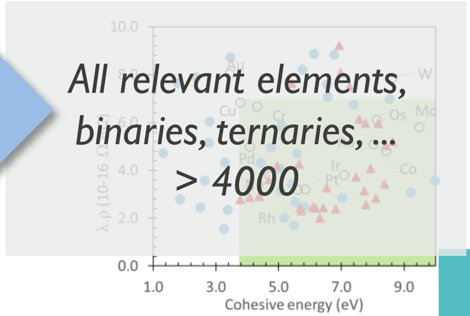
Material screening

Selection of metals for interconnect

0. Problem statement

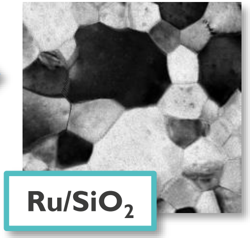


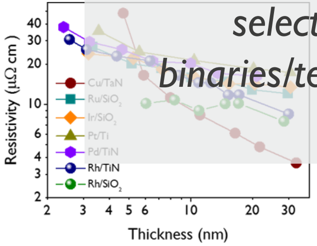
1. Ab initio modeling



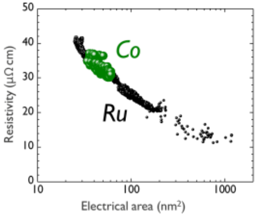
All relevant elements, binaries, ternaries, … > 4000

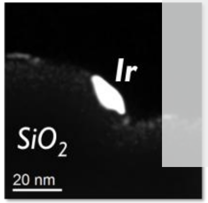
2. Thin film experiments





Ru, Co, Ni, Ir, Rh, Pd, Pt, Nb, Cr, Mo, W, + selected binaries/ternaries





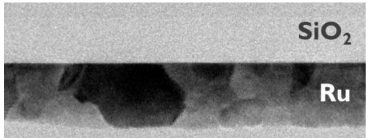
Ru, Co, Ir, Rh, Mo, W

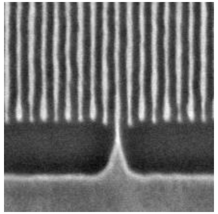
3. Narrow line resistance and scaling potential

4. Process development:

Approach to be used:
Deposition, etch, integration,…

Ru



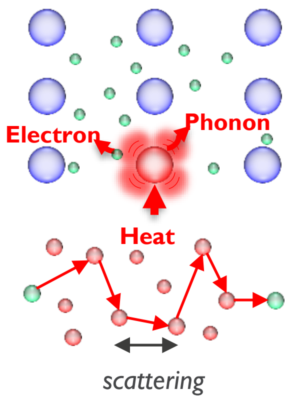


5. Metallization module development

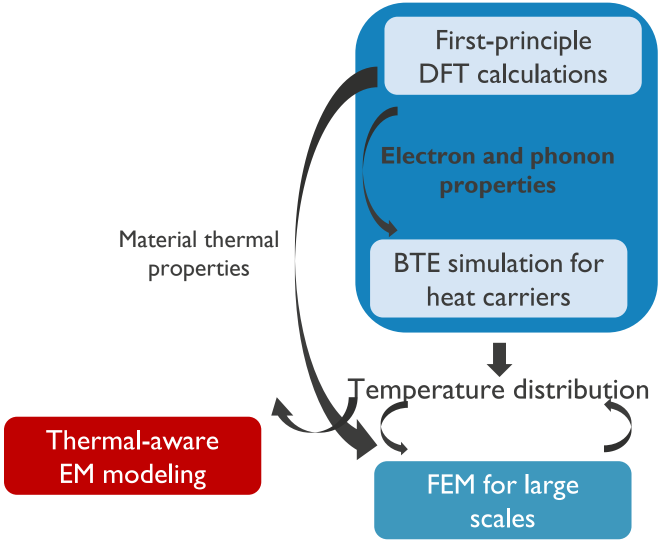
Multiscale modeling

Ex: Atomistic calculations - material thermal properties

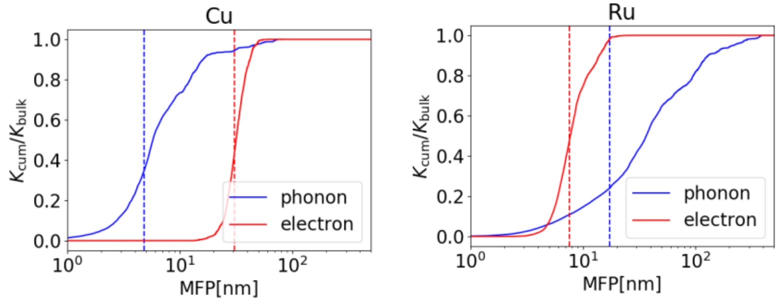
Thermal transport in materials



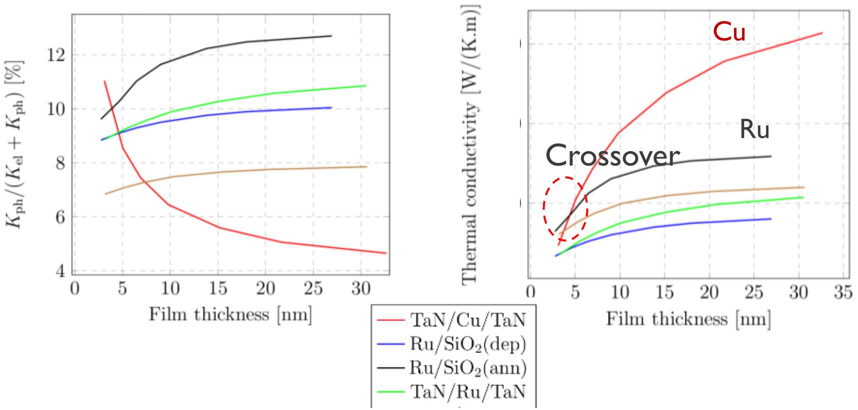
Boltzmann transport equation – Monte Carlo



Bulk thermal conductivities



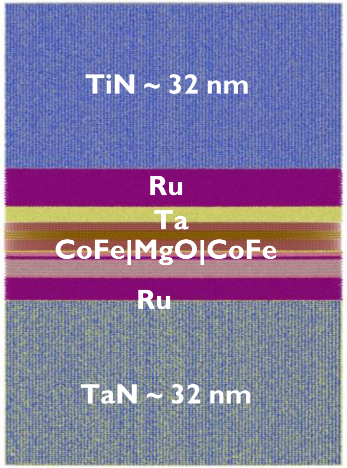
Thin films thermal conductivities



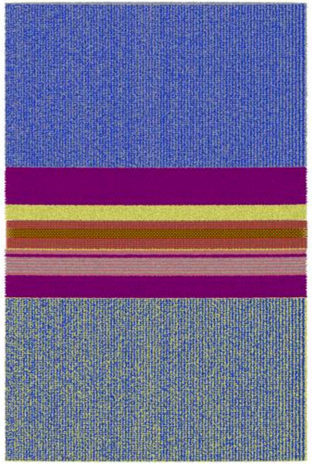
- Electron and phonon properties are calculated from DFT to obtain thermal conductivity.
- Thermal conductivity is modeled in thin film metals using scattering parameters calibrated from elect. measurements.
- Crossover of Cu thermal conductivity with annealed Ru < 5nm.

Multiscale modeling TMR

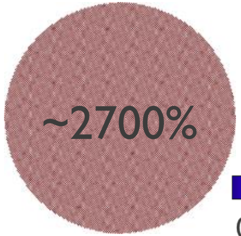
Perfect epitaxial stack
'Romantic' vision

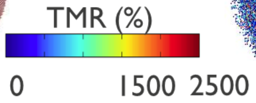


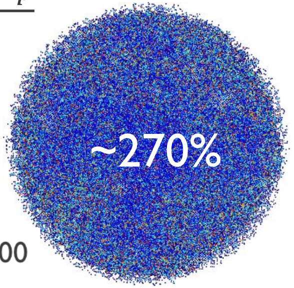
During an elastic deformation
'Atomistic' vision



$$TMR = \frac{R_{ap} - R_p}{R_p}$$



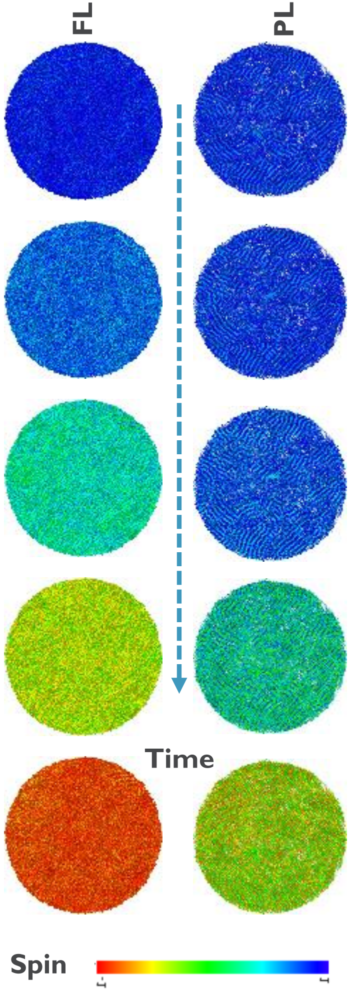




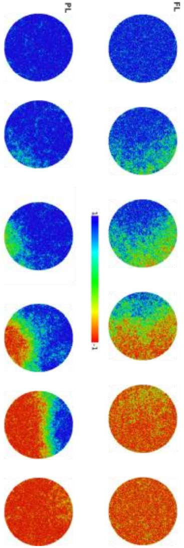
Atomistic (relaxation 1e6 atoms)

Transport (NEGF)

Magnetization switching



Ideal



imec

embracing a better life