Let’s put smart to work

Use Less Materials & Boost Performance

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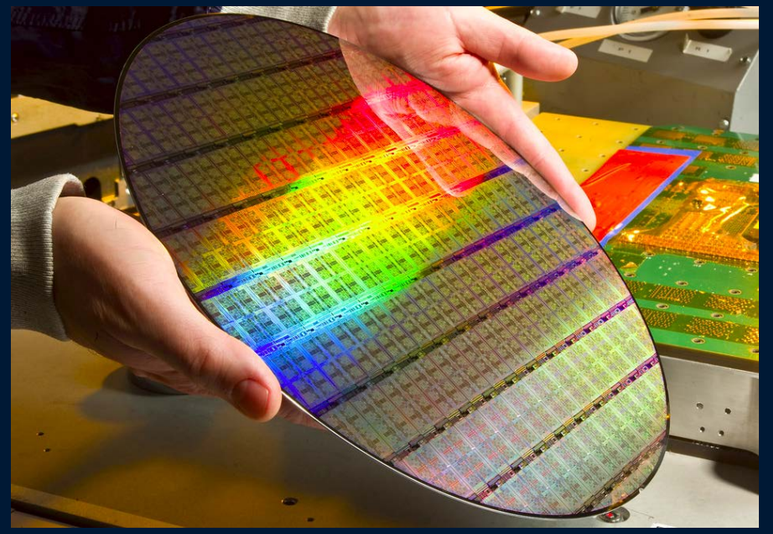
WORLD MATERIALS FORUM

IBM

New Materials Drive Innovation and Business and Create Industries



How can we …

- **Invent faster ?**
- **Use all data available ?**
- **Use less resources ?**
- **Use less materials ?**
- **Use smarter, be smarter ?**

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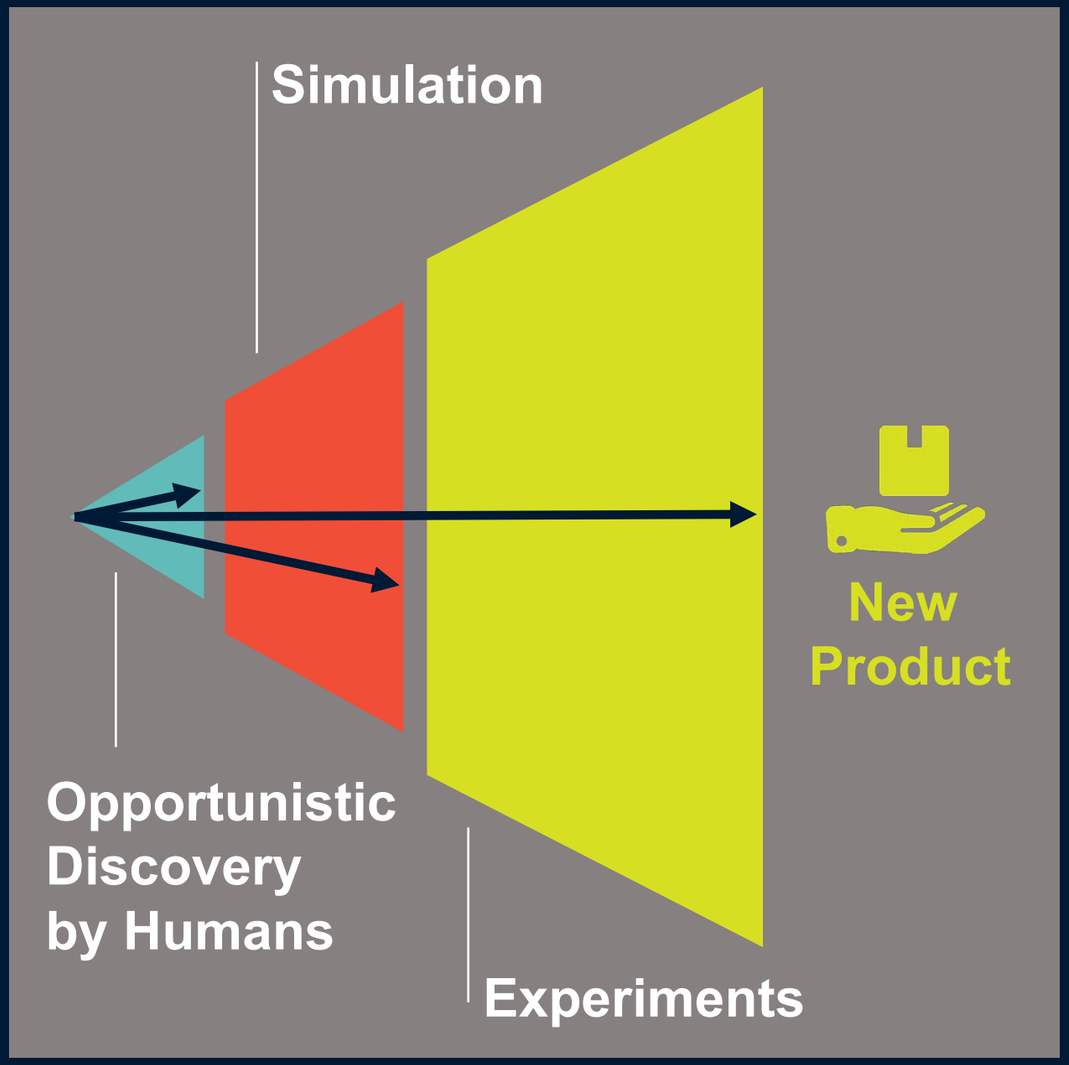
Research & Development Today



- Brute force simulation cannot solve everything.
- Traditional discovery has limits!

➔ We need a new, data driven, holistic approach

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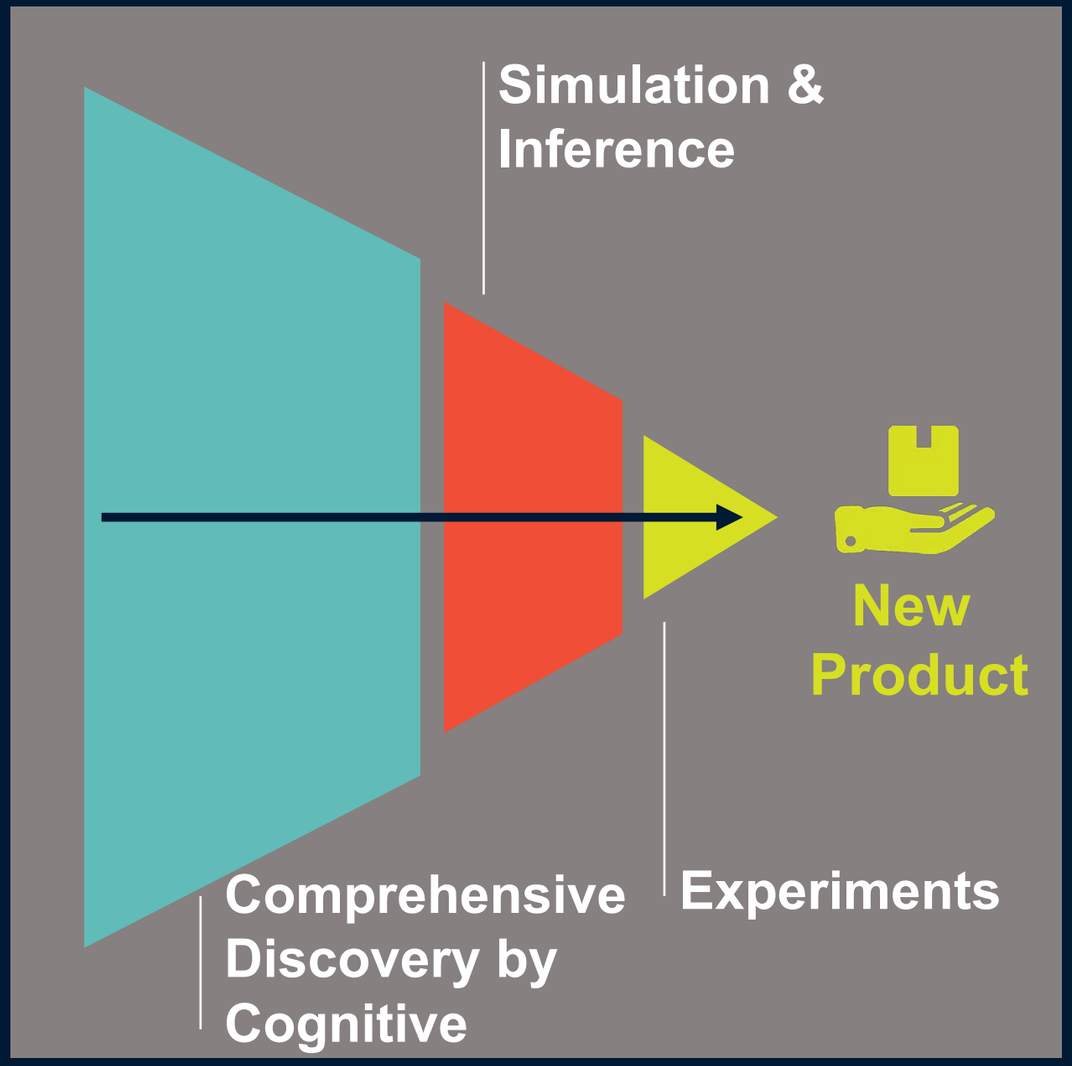
Cognitive Discovery



- **Knowledge based**
- **Uses AI to target which simulations to run & the best way to execute them.**

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Big Data: Scientific Publications

Over 50 million scientific papers have been published

Jinha et al, Learned Publishing 23(3):258-263 · July 2010

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Teach your machine to read papers to accelerate discovery

Performing Quantum Computing Experiments in the Cloud

Simon J. Devitt

Center for Emer

Quantum computing
interest from both the
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anticipated by many, th
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PHYSICAL REVIEW A 94, 012314 (2016)

Experimental test of Mermin inequalities on a five-qubit quan

Daniel Alsina and José Ignacio Latorre

Departament Física Quàntica i Astrofísica, Universitat de Barcelona, Diagonal 645, 080
and Institut de Ciències del Cosmos (ICCUB), Martí i Franquès 1, 08028 Barce

(Received 25 May 2016; published 11 July 2016)

Experimental Comparison of Two Quantum Computing Architectures

N. M. Linke,[1] D. Maslov,[2,3] M. Roetteler,[4] S. Debnath,[1] C. Figgatt,[1] K. A. Landsman,[1] K. Wright,[1] and C. Monroe[1,3,5]

[1] *Joint Quantum Institute and Department of Physics,*

Compressed quantum computation using the IBM Quantum Experience

M. Hebenstreit,[1] D. Alsina,[2,3] J. I. Latorre,[2,3] a

[1] *Institute for Theoretical Physics, University of Innsbruck,*
[2] *Dept. Física Quàntica i Astrofísica, Universitat de Barcelona, Diagon*
[3] *Institut de Ciències del Cosmos, Universitat de Barcelona, Diagonal*

The notion of compressed quantum computation is employed to sim

ProjectQ: An Open Source Software Framework for Quantum Computing

Damian S. Steiger,* Thomas Häner,† and Matthias Troyer‡
Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland
(Dated: December 28, 2016)

We introduce ProjectQ, an op
features a compiler framework
simulator with emulation capab
mation. We introduce our Pyth
provide example implementatio
tum algorithms through simulat
a back-end connecting to the IB
nisms, users can provide back-en
compilation can provide plug-ins
strategies.

Quintuple: a Python 5-qubit quantum computer simulator to facilitate cloud quantum computing

Christine Corbett Moran[a,b,*]

[a] *NSF AAPF California Institute of Technology, TAPIR, 1207 E. California Blvd. Pasadena, CA 91125*
[b] *University of Chicago, 2016 SPT Winterover Scientist, Amundsen-Scott South Pole Station, Antarctica*

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IOP Institute of Physics

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PAPER

Entropic uncertainty and measurement reversibility

Mario Berta[1], **Stephanie Wehner**[2] **and Mark M Wilde**[3,4]

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[2] QuTech, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The N
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rsity, Baton Rouge, LA 70803, USA
hom any correspondence should be addressed.

O Computador Quântico da IBM e o *IBM Quantum Experience*

The IBM Quantum Computer and the IBM Quantum Expe

Alan C. Santos*[1]

de Física, Universidade Federal Fluminense, Niterói, Rio de Ja

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Homomorphic Encryption Experiments on IBM's Cloud Quantum Computing Platform

He-Liang Huang,[1,2] You-Wei Zhao,[2,3] Tan Li,[1,2] Feng-Guang Li,[1,2] Yu-Tao Du,[1,2] Xiang-Qun Fu,[1,2] Shuo Zhang,[1,2] Xiang Wang,[1,2] and Wan-Su Bao[1,2,*]

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n Centre in Quantum Information and Quantum Physics,
y of China, Hefei, Anhui 230026, China
s at Microscale and Department of Modern Physics,

Demonstration of *entanglement assisted invariance* on IBM's Quantum Experience

Sebastian Deffner

Department of Physics, University of Maryland Baltimore County, Baltimore, MD 21250, USA

Leggett-Garg test of superconducting qubit addressing the clumsiness loophole

Emilie Huffman[1,2] and Ari Mizel[1]

oratory for Physical Sciences, College Park, Maryland 20740, USA
nent of Physics, Duke University, Durham, North Carolina 27708, USA

Quantum state reconstruction made easy: a direct method for tomography

R. P. Rundle,[1] Todd Tilma,[2] J. H. Samson,[1] and M. J. Everitt[1,*]

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[2] *Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8550, Japan*

Approximate Quantum Adders with Genetic Algorithms: An IBM Quantum Experience

Rui Li[1], **Unai Alvarez-Rodriguez**[2], **Lucas Lamata**[2], **and Enrique Solano**[2,3]

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ABSTRACT

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Reading papers like a materials scientist

Polymer 79 (2015) 255–267

Contents lists available at ScienceDirect

Polymer

journal homepage: www.elsevier.com/locate/polymer

Water soluble, biodegradable amphiphilic polymeric nanoparticles and the molecular environment of hydrophobic encapsulates: Consistency between simulation and experiment

Robert D. Miller*, Rosmadi M. Yusoff [1], William C. Swope, Julia E. Rice, Amber C. Carr [2], Amanda J. Parker [3], Joseph Sly [4], Eric A. Appel [5], Timothy Nguyen [6], Victoria Piunova

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Modeling and simulation

ABSTRACT

Star polymers with a crosslinked nanogel core constitute an unusual class of polymers with many arms emanating from the functionalized core. Although the core is usually hydrophobic, the arms can be hydrophobic, hydrophilic or amphiphilic. We describe the synthesis of biodegradable nanogel core stars which are largely water soluble and use encapsulated pyrene fluorescence to probe the environment both in aqueous solution and in solid thin films. In spite of the expected hydrophobic nature of the inner portions, the encapsulated pyrene environment seems quite polar. Although the molecular environment based on the pyrene fluorescent probe of the inner aliphatic polyester regions is more polar than expected for an aliphatic polyester, the molecular environment of the encapsulated probe in aqueous solution is influenced by the proximity of water even though simulations suggest that water excursions into the inner regions of the hydrophobic core area are rare and transient. NMR studies in water show the disappearance of the arm polyester signals. This and the pyrene environmental probe studies are consistent with collapse of the inner polyester regions and localization of the probe at or near the hydrophobic/hydrophilic interface as suggested in the simulations. This study has implications for the encapsulation of strongly hydrophobic cargos barring some loosening of the collapsed core by sterically-demanding substituents, increased hydrophobicity and/or some optimized specific interactions of the cargo with the core.

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1. Introduction

Many therapeutic drugs and food supplements are quite hydrophobic and require a delivery vehicle for application in aqueous solution. Increasingly, these agents are nanostructured and often include nanoparticle-like entities such as lipid-based systems [1], dynamic micelles, covalently crosslinked or non-covalently stabilized micelles [2], polar and nonpolar polymeric nanoparticles [1a,d,3] which can be either biodegradable or not, inorganic nanoparticles including ceramic, semiconductor, metallic nanoparticles both magnetic and non-magnetic [4], etc. We and others have been studying a class of materials, which we describe as nanogel core star polymers [5] that have a small crosslinked core from which arms and other functionality protrude. Some of these materials are amphiphilic, unimolecular micelles with a small hydrophobic internal core which is crosslinked, often an additional hydrophobic section provided by the arms as well and an outer corona which is polar to interact with the aqueous environment and stabilize the particle in water. The result is a unimolecular micelle that is not in traditional dynamic equilibrium with its components, has no critical micelle concentration and is hence stable to extreme dilution. These structures can be biostable, biodegradable or biocompatible depending on the components of

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[6] Gilead Sciences Inc., 333 Lakeside Dr, Foster City CA, 94404-1147.

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data from text

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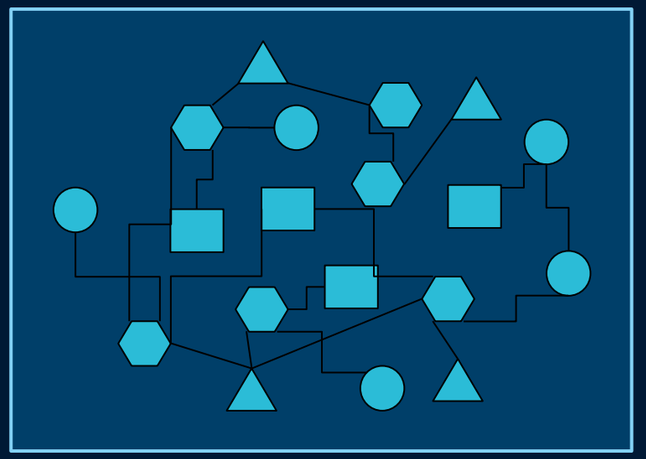
semantic analysis

MATERIALS KNOWLEDGE GRAPH



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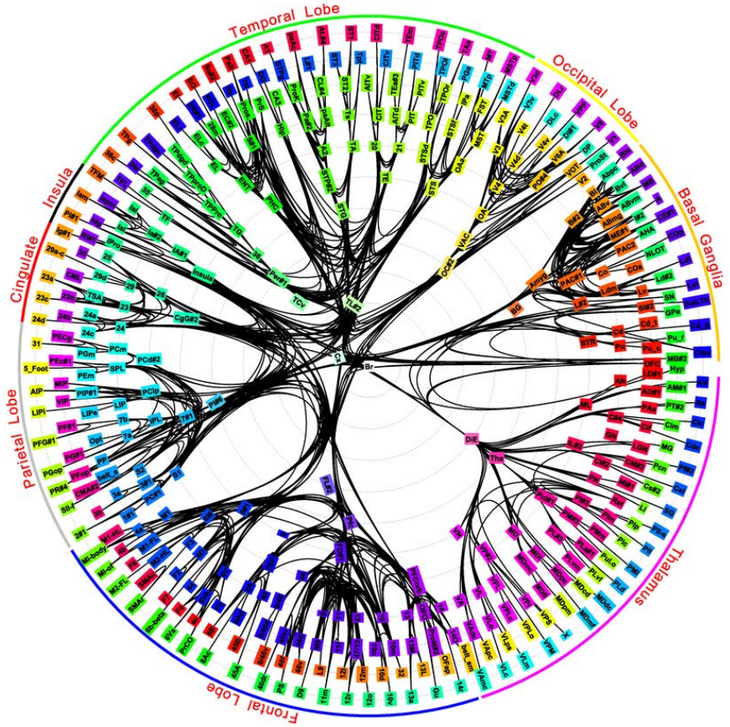
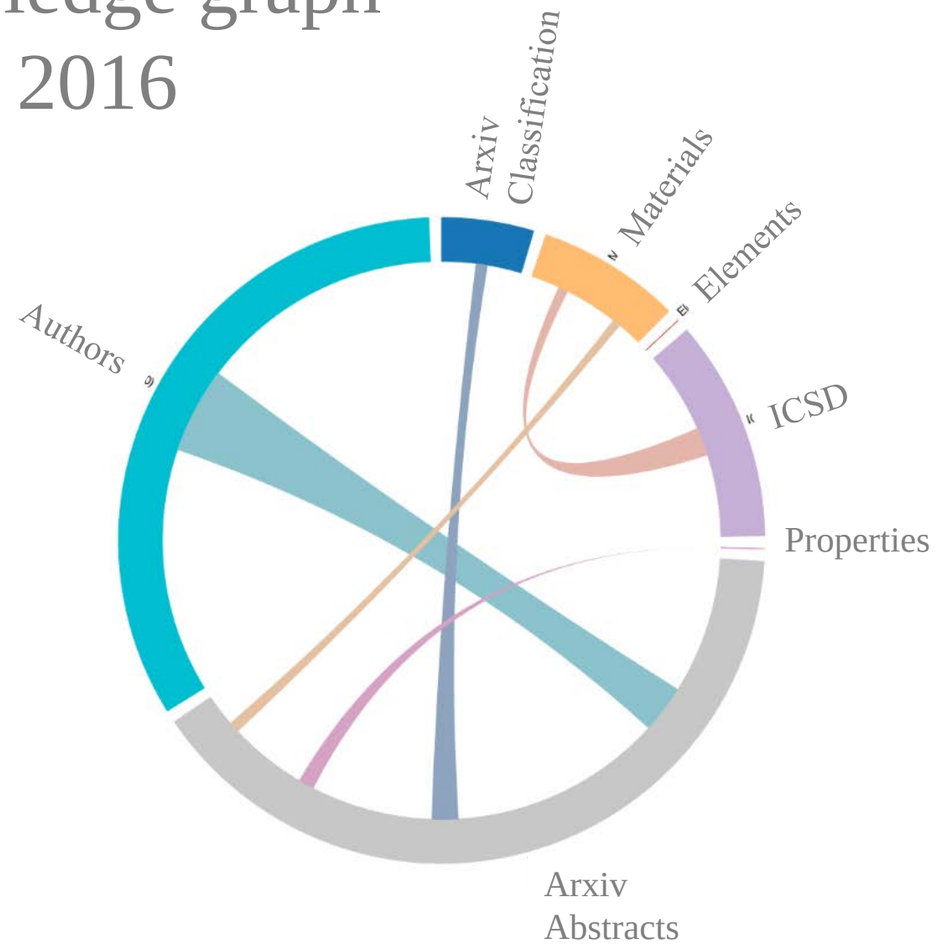
Macaque brain connectivity network IBM, 2010



Each color is a different anatomical area
Black lines are the connections

383 nodes, 6602 edges,
person-decades

Materials knowledge graph IBM, 2016



>1M nodes, >100k edges,
600k documents, 1 node-hour

III-V Materials – A Necessity and Opportunity

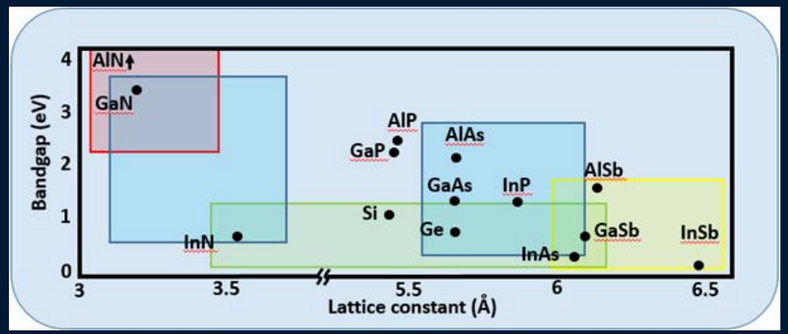
SOI

Copper

SiGe

High-k

- **Semiconductor Industry quests new materials for continued progress**
- **III-V Semiconductors**
  - **High electron mobility**
  - **Direct bandgap**
  - **Allow bandgap engineering and heterostructures**
- **Improved Devices – Alternative Devices – Additional Functionalities:**
  - RF devices
  - High performance n-FETs
  - Optoelectronics: Lasers, LEDs, photodetectors
  - Solar Cells
  - Devices for Quantum Computing



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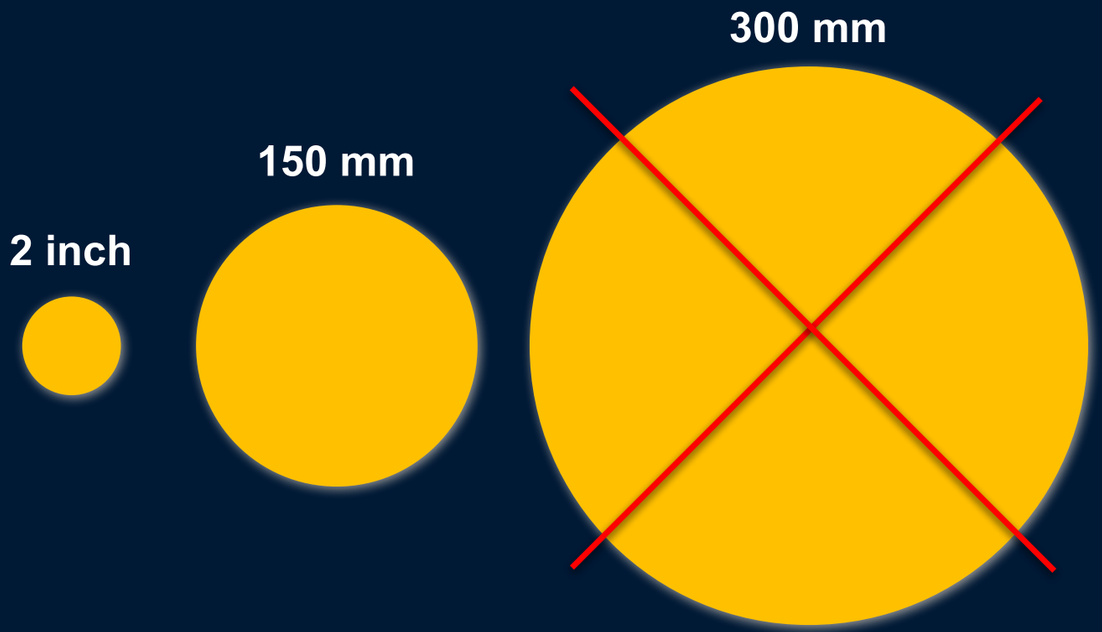
But …

- **III-V wafer size and availability (<6 inch)**
- **III-V wafer cost (e.g. 6 inch GaAs ca $200)**



Therefore:

- **Applications limited**
- **Economy of scale limited**

Needed:

- **Integration on Si**
- **Smarter way of using III-V materials**

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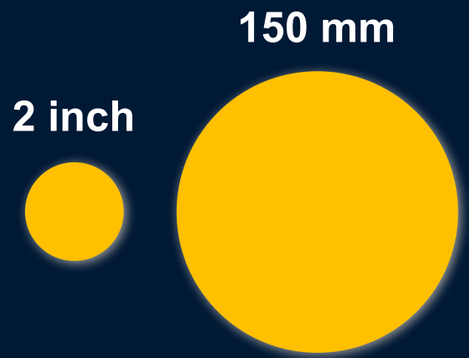
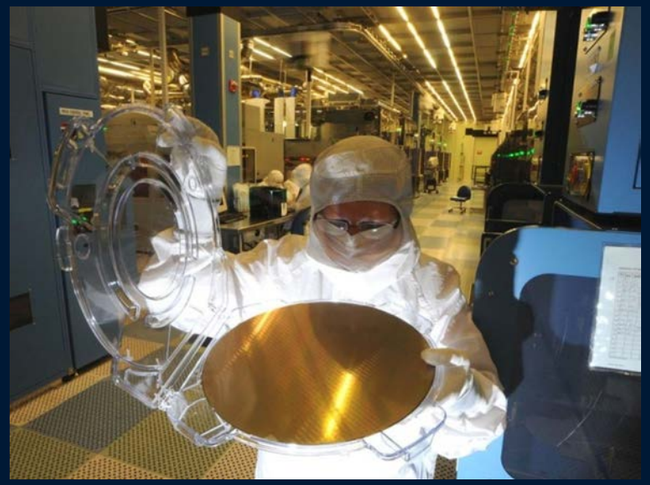
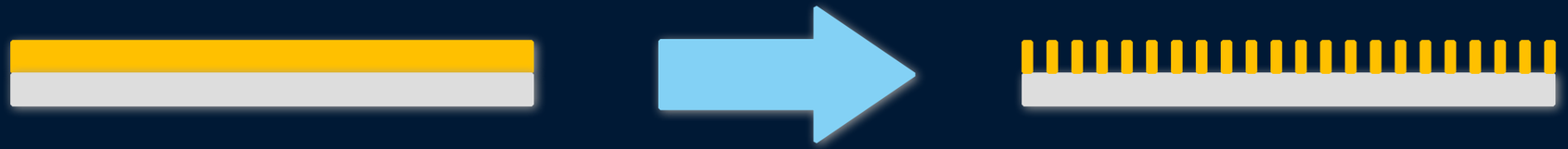
Use Less – Use Smarter







And Boost Performance

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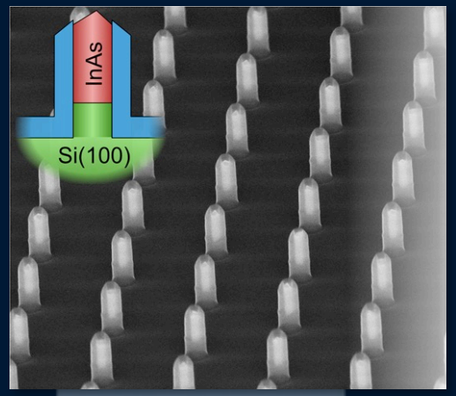
New Growth Technique – Template Assisted Selective Epitaxy

Vertical nanowires

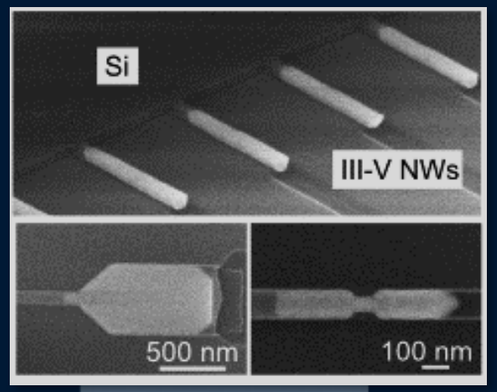


Borg et al. Nano Lett. 2014

High-density electronics

Solar

Horizontal nanostructures



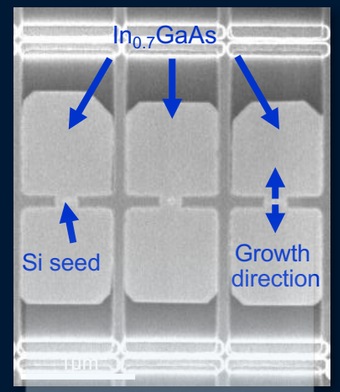
Schmid et al. APL. 2015

CMOS

Low-power electronics

Photonics

Planar micro-layers



Czornomaz et al. VLSI 2015

CMOS

Lasers

➔ **Use III-V only were needed on Silicon**

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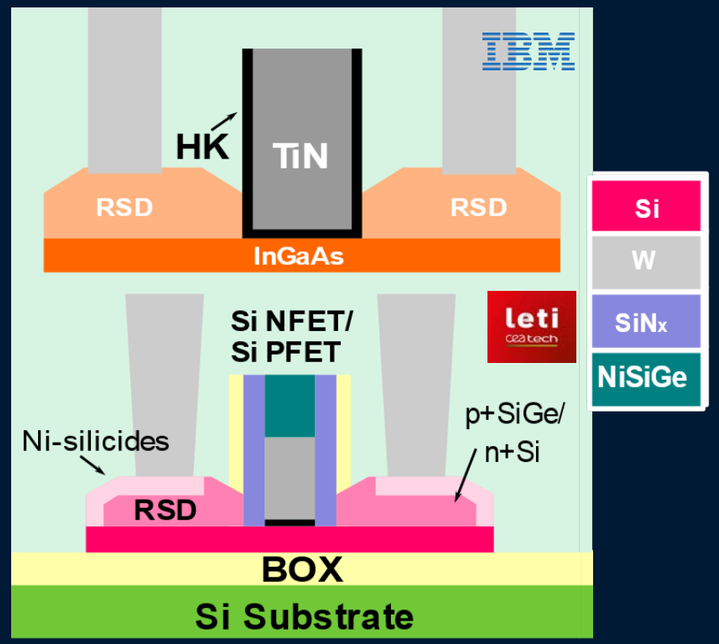
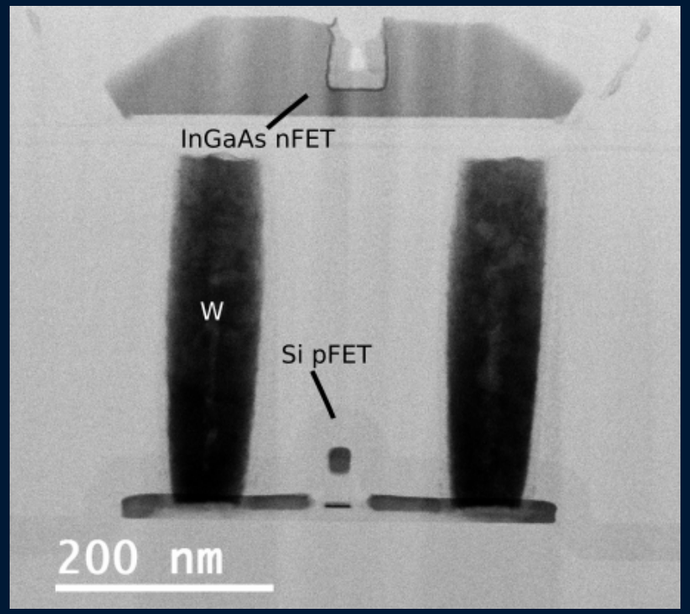
Example: Electronics Applications





- InGaAs FinFETs **integrated** on FDSOI Si CMOS
- No degradation of Si CMOS performance
- **Bottom-up approach**: growing III-V only where needed
- **Record-high I_{ON}** of 170 µA/µm for integrated III-V FETs achieved at scaled gate length (30nm)

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Example: III-V Solar Cells

- **Si solar cells** broadly used
  - Efficiency: theoretical limit 29%, Commercial: 25 %
- **III-V solar cells** for special applications (space mission, concentrator photovoltaics)

Advantages III-V semiconductors:

- Band gap direct & tunable
- **Multi-junction solar cells** possible
  - Stacking of materials with different bandgap
  - Harvest broader spectrum of sun light
  - Quadruple-junction solar cell: GaInP/GaAs/GaInAsP/GaInAs
  - World-record: **46%** (4 cells)
- **But**
  - **High cost** of III-V materials
  - **Size and cost** of III-V **substrates**
- **Current solution:**
  - **Small device** combined with **light concentration**
  - Cost of light integrating systems, cooling system, etc.

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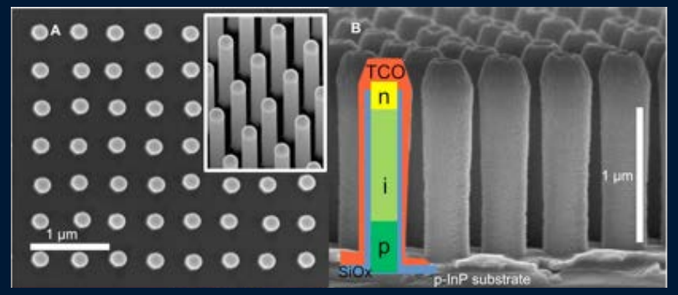
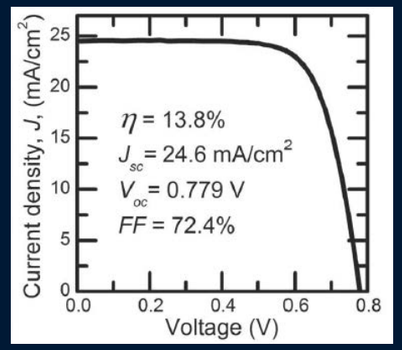
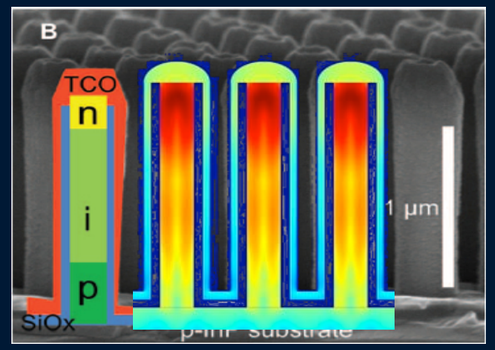
III-V Nanowires for Solar Cells

- III–V NWs allow a **significant reduction** in material needed
- Have the potential to **exceed the performance** of conventional devices

InP Nanowire Array Solar Cells







J. Wallentin et al. SCIENCE 339, 1057, 2013

- InP NW solar cell *on III-V substrate*
- **High absorption:** NW array absorbs more light with less material due to **resonant light trapping**
- NWs (180nm diameter) covering **12% of surface**
- **Absorbs 20x more light** than same volume planar III-V film
- III-V NW cells need only about 1-2µm length (Si >100x more)
- **BUT** on III-V substrate

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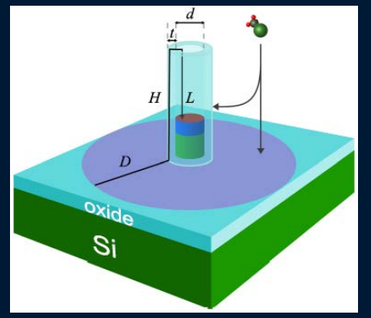
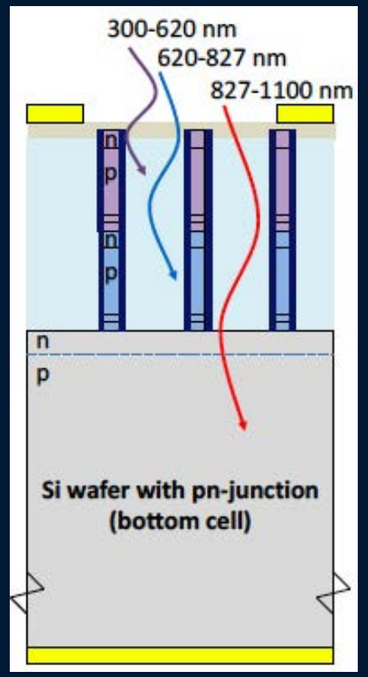
III-V Nanowires on Silicon for Solar Cells

- III–V Nanowires combined with Si PV technology have the potential of simultaneously allowing **very high performance, efficient use of materials, and low cost**.



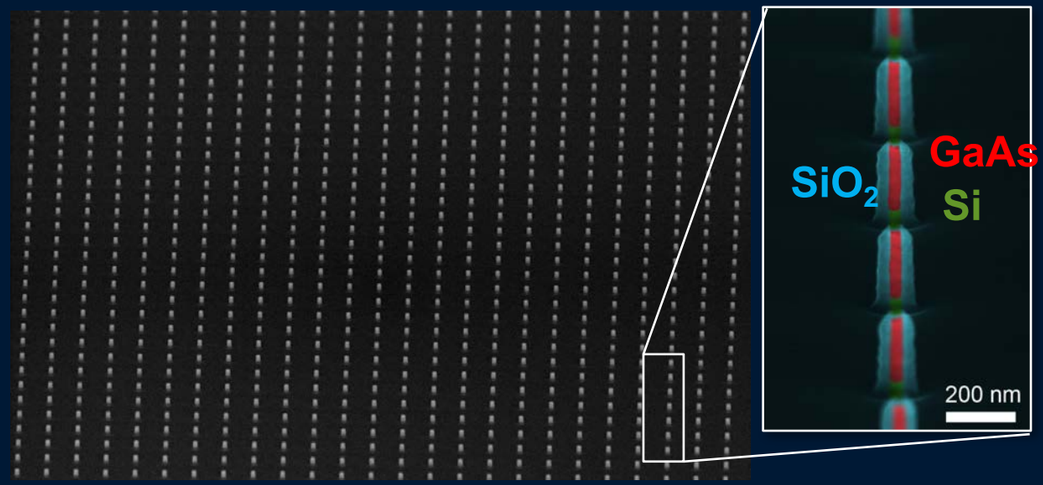
III-V Nanowire Solar Cell combined with Si cell



Standard Si PV combined with top III-V NW
(upper NW cell can contain two bandgaps)
➔ three bandgap solar cell technology, with **theoretical maximum efficiency of ≈ 50%**

- **Ultra-low III-V materials use**:
  about 1 g of III-Vs for a 1m^2 solar panel
- Panel **efficiency** can be **increased** by
  - **35%** for high-end PV-cells
  - **>60%** for low-end PV-cell technology
  - (for a small cost increase (≈15%))

GaAs Nanowire grown on Si by TASE



NANO TANDEM
Funding: GA 641023 H2020

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Let’s put smart to work

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