What ever happened to combinatorial materials discovery?
by Geoffrey Ozin | Jun 17, 2020

https://www.advancedsciencenews.com/what-ever-happened-to-combinatorial-materials-discovery/?elq_mid=45762&elq_cid=2081930&elqCampaignId=28729&utm_campaign=28729&utm_source=eloquaEmail&utm_medium=email&utm_content=EMAIL%20Advanced%20Science%20News%20DE%201ST%20200623%20GSALL&elqTrackId=92d11a8791904e9ebd0a9d2ba84be44c&elq=46016d0a414a42e1afa58a4673a5fd07&elqaid=45762&elqat=1&elqCampaignId=28729

If we have 5 professional baseball teams

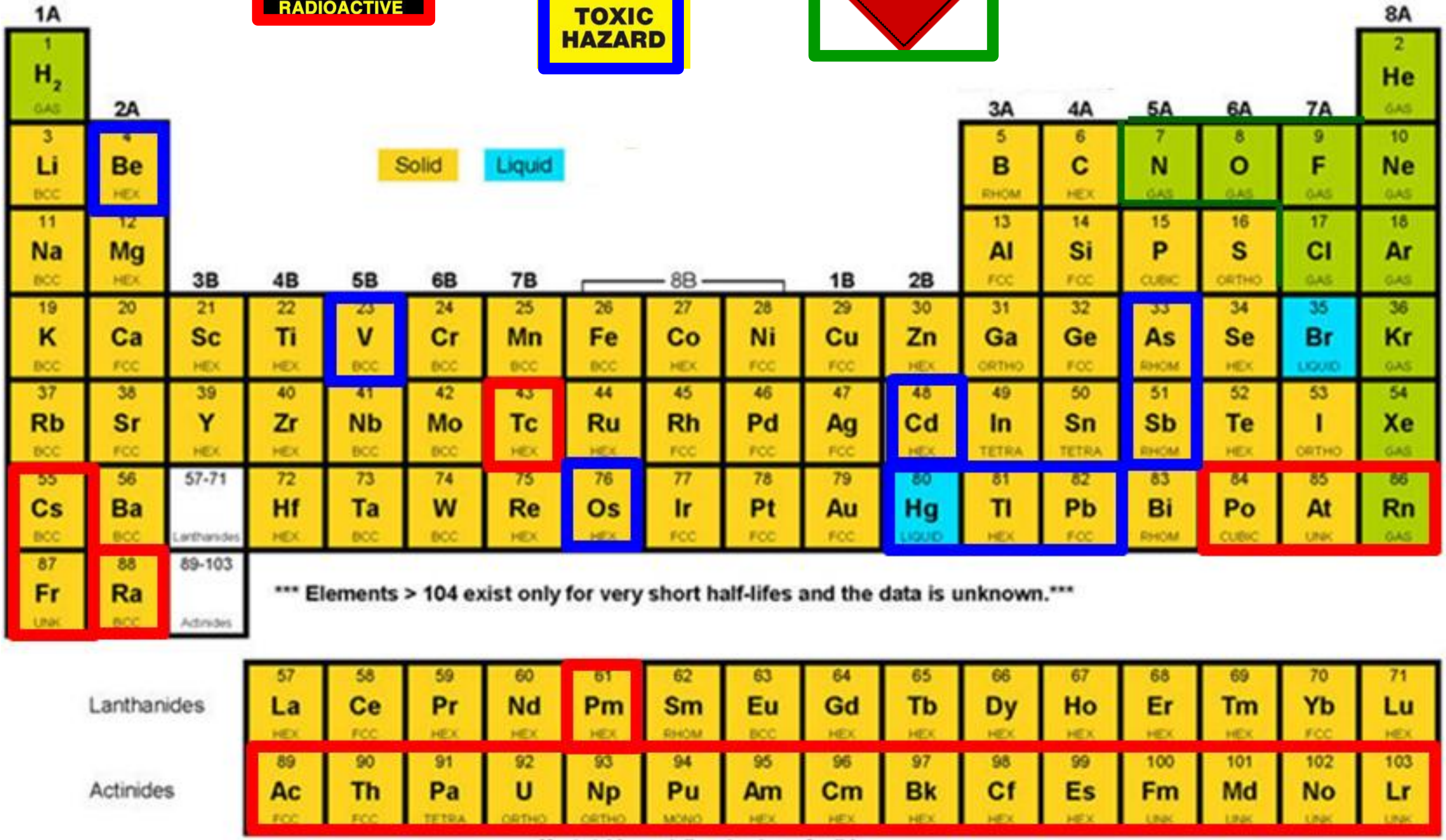
$$C^{5}_{2} = \frac{5!}{2!\ (5-2)!}$$

$$= 10$$


CAUTION
RADIOACTIVE


TOXIC
HAZARD


FLAMMABLE GAS


1A
2A
3A
4A
5A
6A
7A
8A
3B
4B
5B
6B
7B
8B
1B
2B
Solid
Liquid
1 H2 GAS
2 He GAS
3 Li BCC
4 Be HEX
5 B RHOM
6 C HEX
7 N GAS
8 O GAS
9 F GAS
10 Ne GAS
11 Na BCC
12 Mg HEX
13 Al FCC
14 Si FCC
15 P CUBIC
16 S ORTHO
17 Cl GAS
18 Ar GAS
19 K BCC
20 Ca FCC
21 Sc HEX
22 Ti HEX
23 V BCC
24 Cr BCC
25 Mn BCC
26 Fe BCC
27 Co HEX
28 Ni FCC
29 Cu FCC
30 Zn HEX
31 Ga ORTHO
32 Ge FCC
33 As RHOM
34 Se HEX
35 Br LIQUID
36 Kr GAS
37 Rb BCC
38 Sr FCC
39 Y HEX
40 Zr HEX
41 Nb BCC
42 Mo BCC
43 Tc HEX
44 Ru HEX
45 Rh FCC
46 Pd FCC
47 Ag FCC
48 Cd HEX
49 In TETRA
50 Sn TETRA
51 Sb RHOM
52 Te HEX
53 I ORTHO
54 Xe GAS
55 Cs BCC
56 Ba BCC
57-71 Lanthanides
72 Hf HEX
73 Ta BCC
74 W BCC
75 Re HEX
76 Os HEX
77 Ir FCC
78 Pt FCC
79 Au FCC
80 Hg LIQUID
81 Tl HEX
82 Pb FCC
83 Bi RHOM
84 Po CUBIC
85 At UNK
86 Rn GAS
87 Fr UNK
88 Ra BCC
89-103 Actinides
*** Elements > 104 exist only for very short half-lifes and the data is unknown.***
Lanthanides
57 La HEX
58 Ce FCC
59 Pr HEX
60 Nd HEX
61 Pm HEX
62 Sm RHOM
63 Eu BCC
64 Gd HEX
65 Tb HEX
66 Dy HEX
67 Ho HEX
68 Er HEX
69 Tm HEX
70 Yb FCC
71 Lu HEX
Actinides
89 Ac FCC
90 Th FCC
91 Pa TETRA
92 U ORTHO
93 Np ORTHO
94 Pu MONO
95 Am HEX
96 Cm HEX
97 Bk HEX
98 Cf HEX
99 Es HEX
100 Fm UNK
101 Md UNK
102 No UNK
103 Lr UNK

C^{60}_{2} ≈ **1800** binary compounds

C^{60}_{3} ≈ **35,000** ternary compounds

C^{60}_{4} ≈ **500,000** quaternary compounds

Combinatorial Methodology


MANY AT A TIME Program head Andreas Marzinik (front to back) and lab specialists Raphael Gattlen and Urs Rindisbacher of Novartis Pharma AG, Basel, Switzerland, pipette coupling reagent into 96-well reaction blocks.

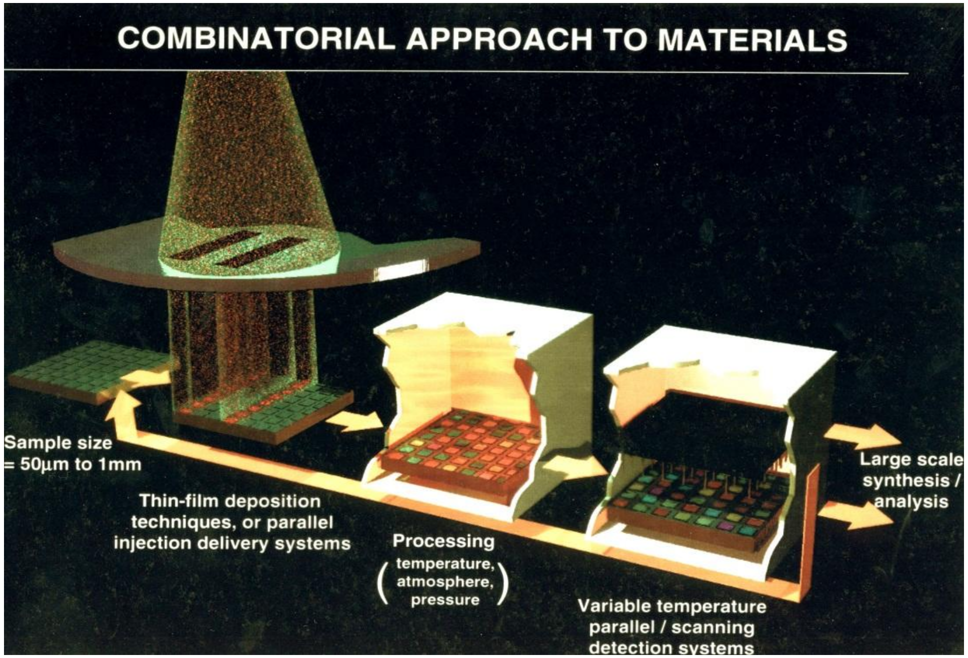
COMBINATORIAL CHEMISTRY

Chemical & Engineering News, August 2001

- First applied in the pharmaceutical industry
- In 1993, Peter Schultz first extended this technique to functional inorganic materials.
- Dielectrics/ferroelectrics
  Ferromagnetics
  Superconductors
  Colossal magnetoresistive
  Ferromagnetic semiconductors
  Polymers
  Luminescent materials

Now: Advanced Gate Stacks

Combinatorial Thin Film Experiments



- Synthesis of a large number of different compositions on one chip at one time.
- Observation of trends.
- Rapid screening (finding the “sweet spot” of the response urface).
- Structure-composition-property relationship.

Ink-jet liquid-dispensing System

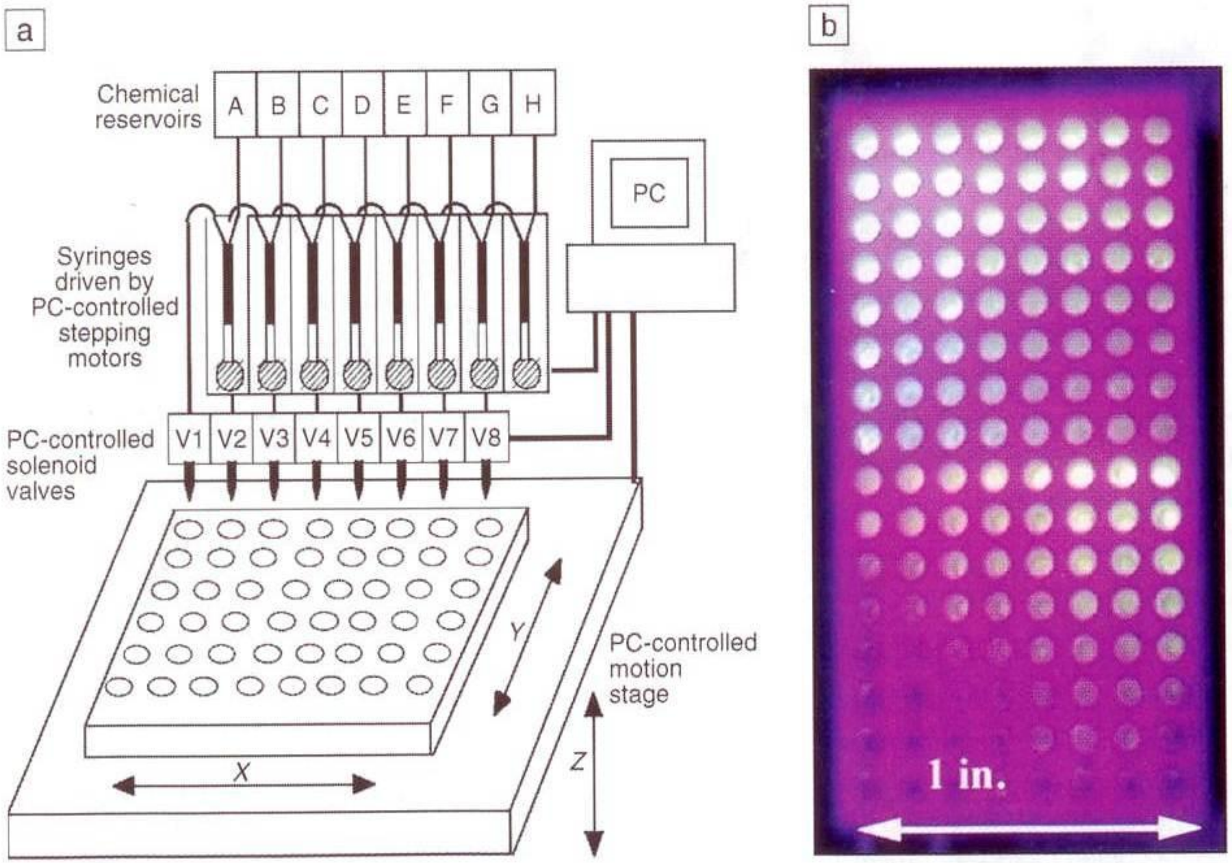
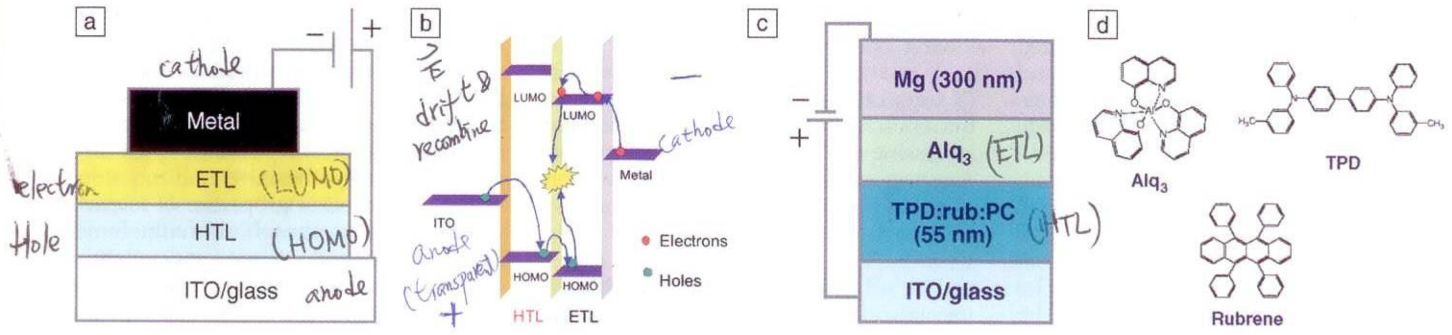


Figure 2. (a) Schematic illustration of an automated liquid-dispensing system for making powder phosphor libraries. (b) Photoluminescence image of a powder phosphor library: $(Y_xCe_{0.06}A_{1-x})_3(Al_yGa_{1-y})_5O_{12}$, excited with a uniform long-wavelength UV (365 nm) field.

Organic Light-emitting Devices



ETL effect

Thickness effect

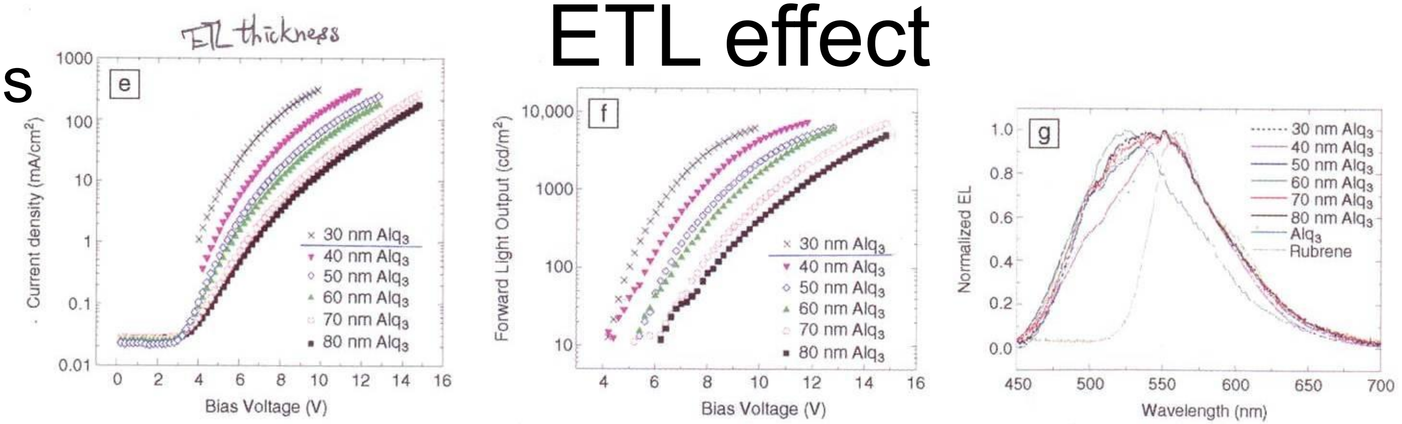
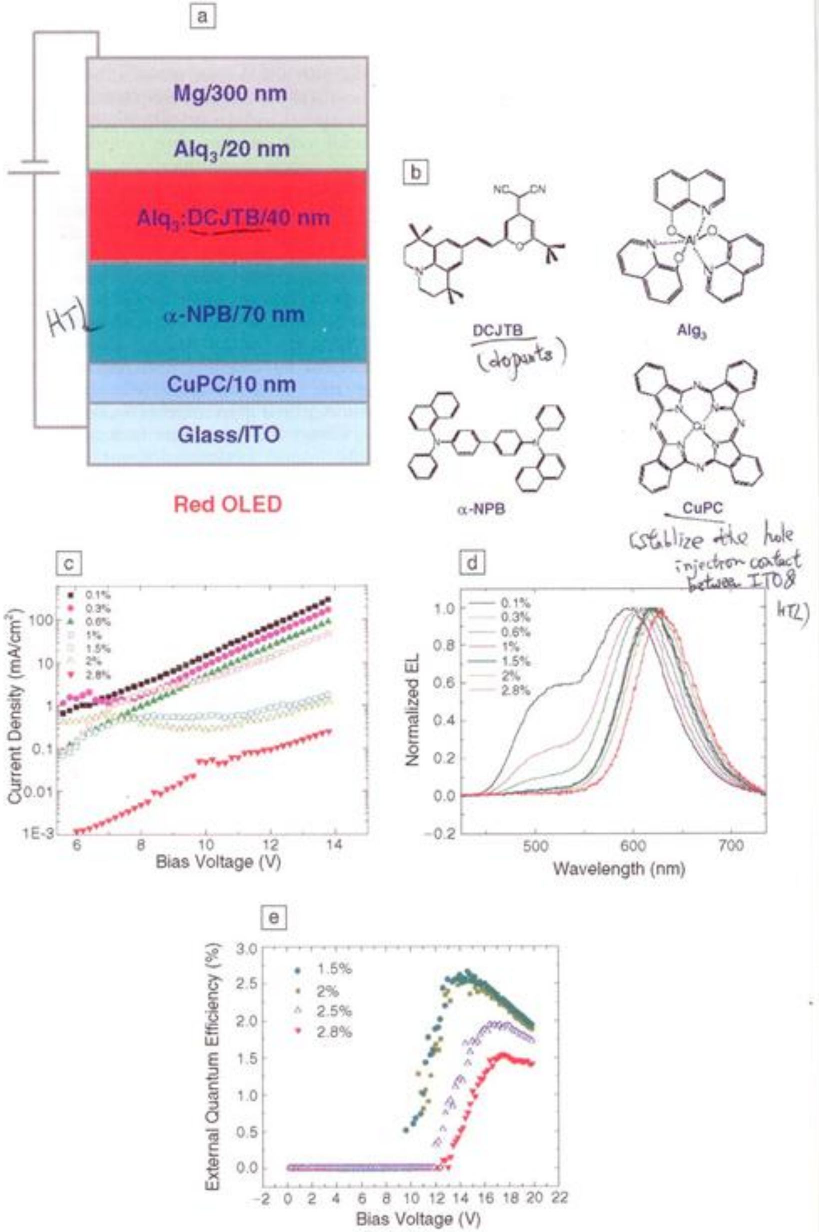


Figure 3. (a) Typical structure of an organic light-emitting device (OLED). ETL stands for electron-transport layer, HTL stands for hole-transport layer, and ITO is indium tin oxide. (b) Simplified energy diagram for an OLED with two organic layers. LUMO stands for the lowest-unoccupied molecular orbital, and HOMO stands for the highest-occupied molecular orbital. (c) Device cross section (layer thickness is not drawn to scale). (d) Chemical structure of the organic molecules used in OLED fabrication. (e) Current density versus forward-bias voltage for OLEDs with ETL thicknesses of 30 nm, 40 nm, 50 nm, 60 nm, 70 nm, and 80 nm, respectively. (f) Forward light output of the OLEDs with various ETL thicknesses versus bias voltage. (g) Normalized electroluminescence (EL) of the OLEDs with different Alq_3 (8-tris-hydroxyquinoline aluminum) thicknesses. The figure also shows the emission spectra of Alq_3 and rubrene thin films.

ETL effect

Dopant effect



9. * layers by CVD : MOS transistor structure

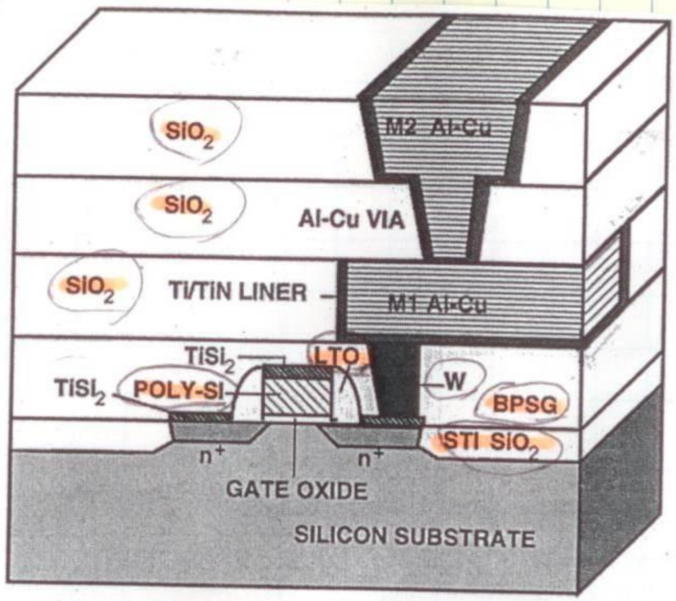


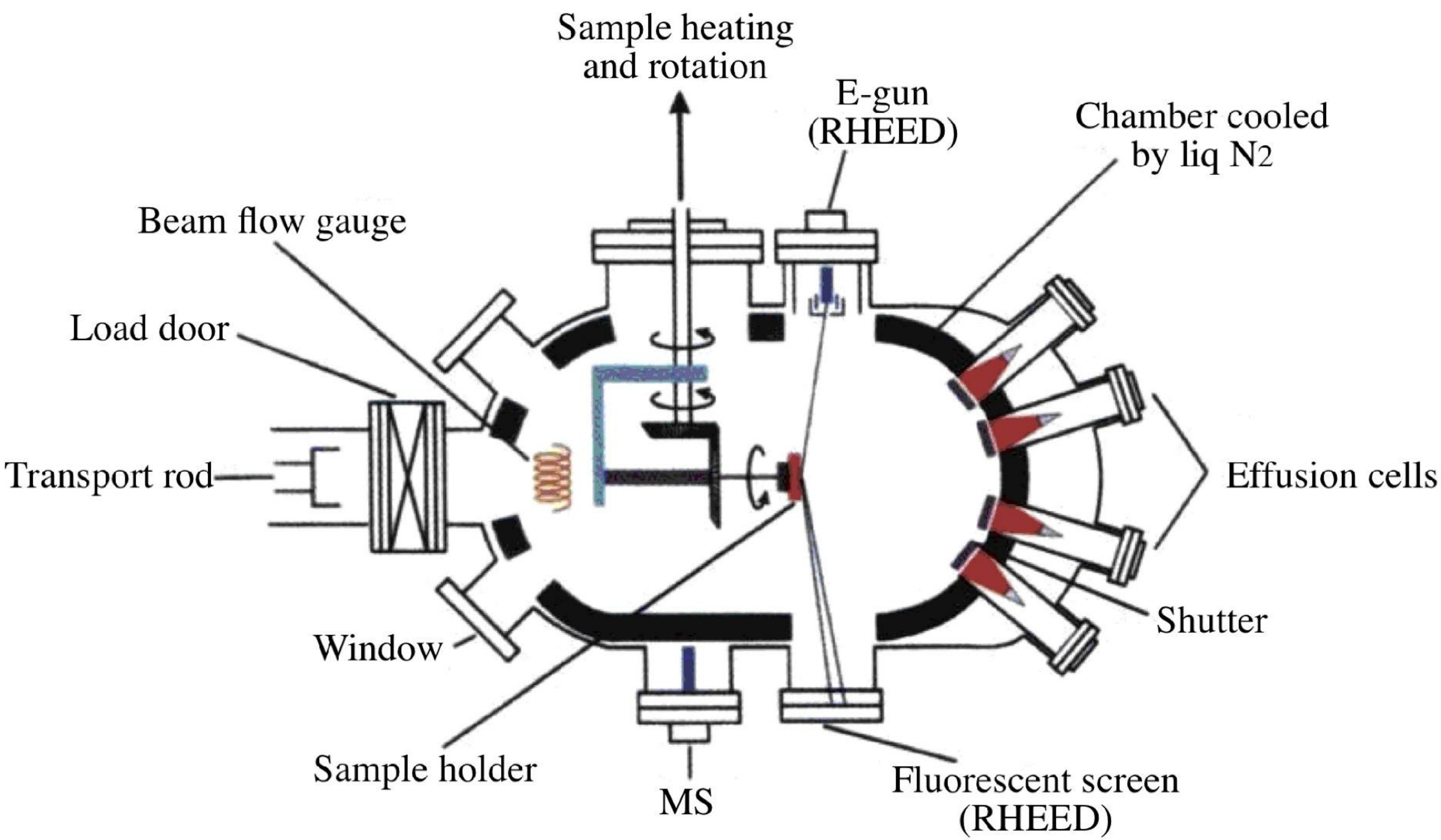
Figure 6-1 Schematic cross-sectional view of an MOS transistor structure with multilevel metallization scheme. Film materials deposited by CVD are indicated in the text. *Note:* LTO = low temperature oxide, BPSG = borophospho-silicate glass, STI = silicon trench insulator. After K. P. Rodbell, IBM, T. J. Watson Research Division.

P.278

poly-Si
various SiO_2 films
low-temp. oxide (LTO)
borophospho-silicate glass (BPSG)
silicon trench insulator (STI)
phosphosilicate glass (PSG)
SiO_2 films precursors : CVD (refer to chap.5, SZE)

12. advantages
* produce a large variety of films and coatings of metals, semiconductors, inorganic / organic compounds either in crystalline or vitreous form

Molecular Beam Epitaxy



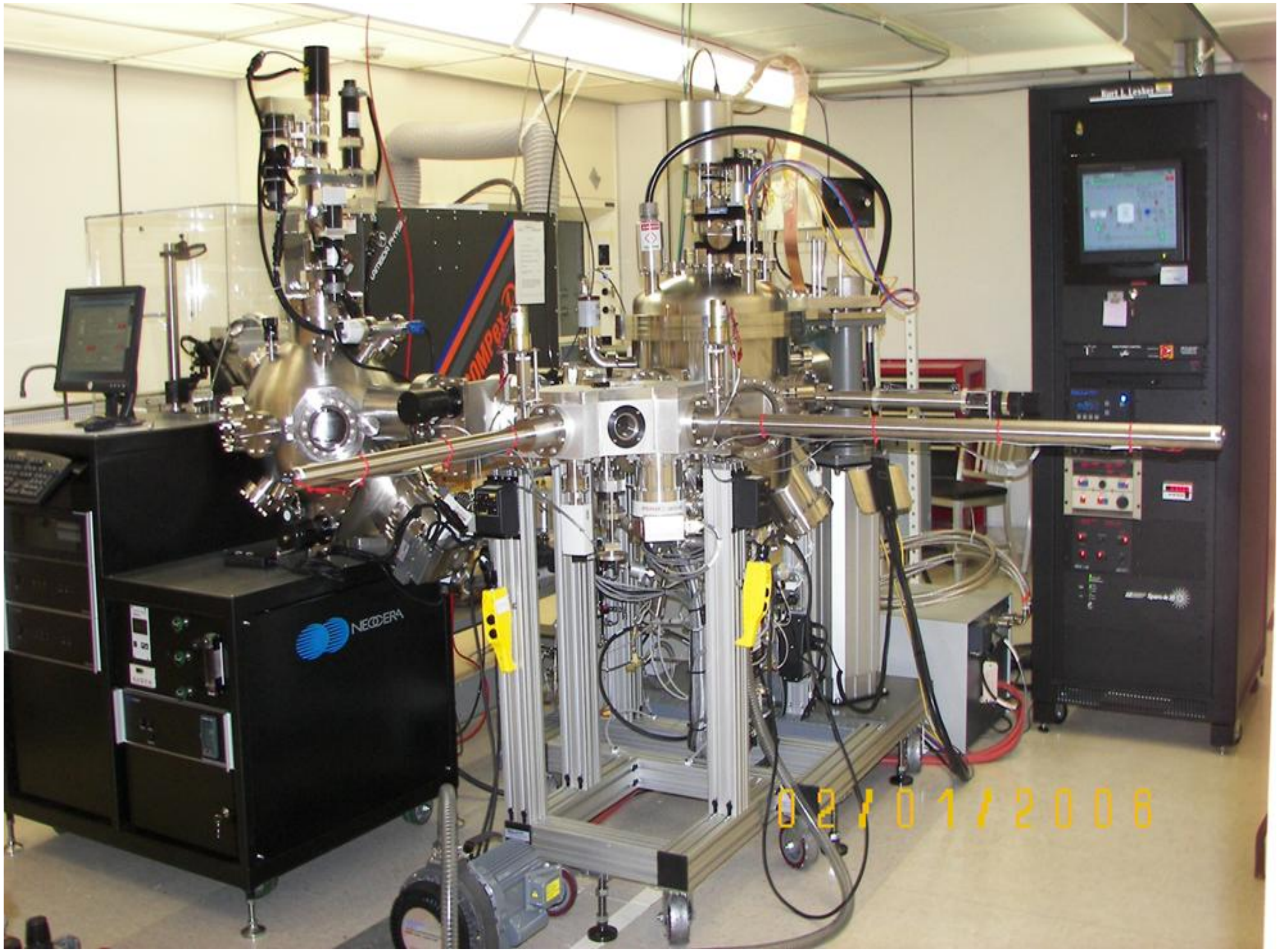
http://archive.cnx.org/contents/0b2614e4-aa98-49c1-bf50-1db3ee3c5ecd@2/molecular-beam-epitaxy

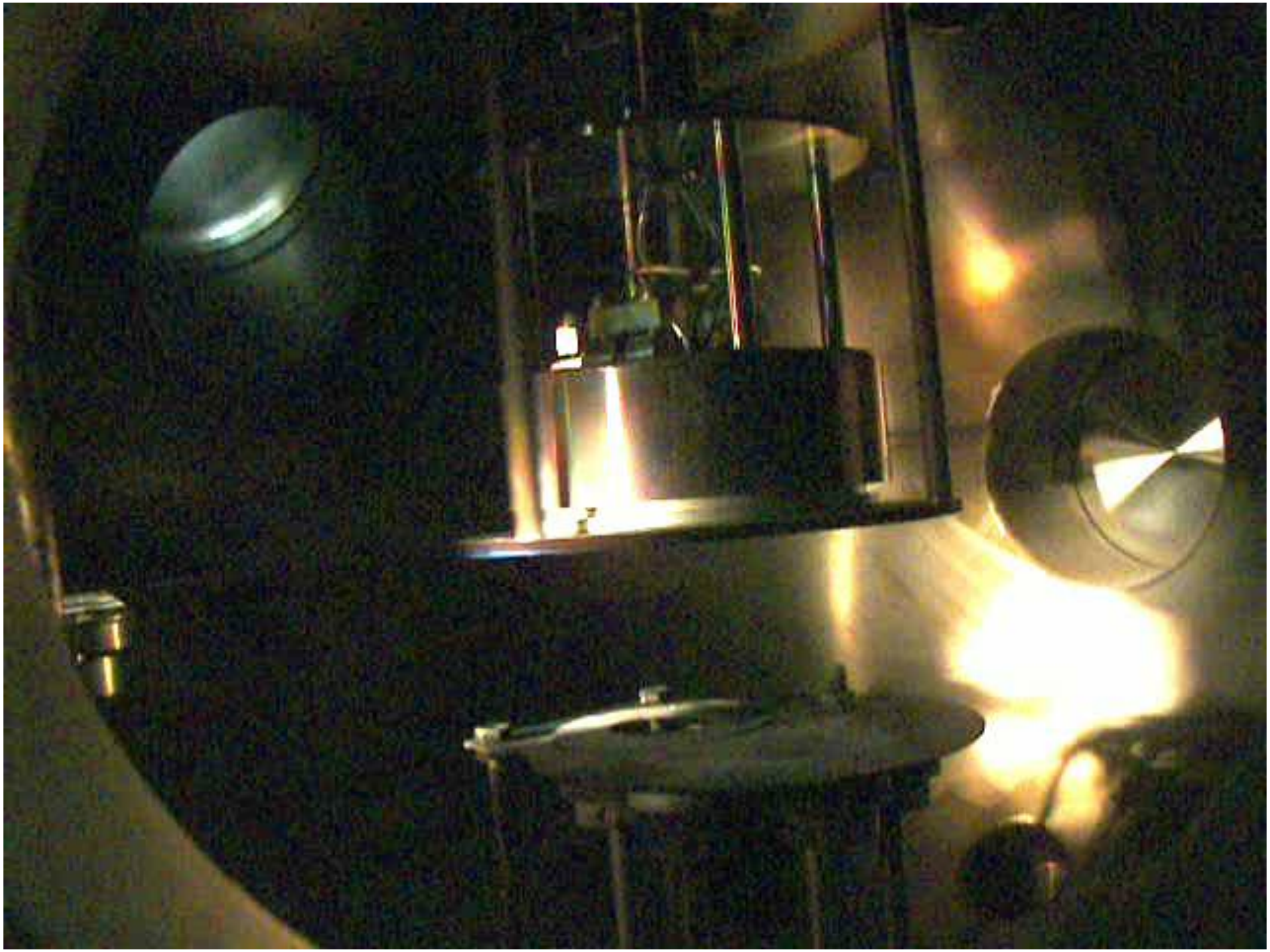
Miniature Knudsen-Cell (K-Cell)

http://www.tectra.de/k-cell.htm

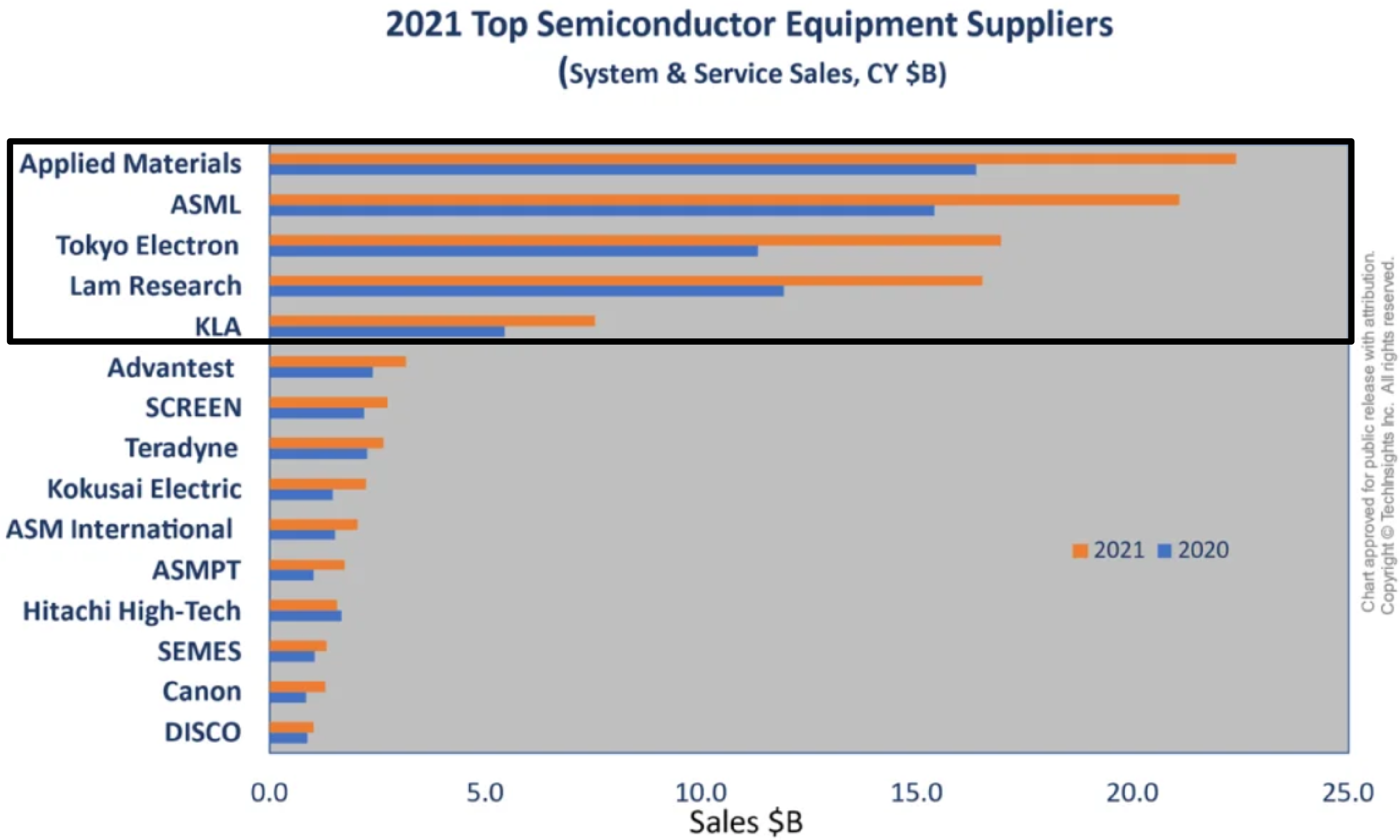
Vacuum levels

- **Atmospheric pressure: 760 Torr**
- Vacuum cleaner: approximately 600 Torr
- Near earth outer space: approximately 10^{-6} Torr
- **Cryopumped MBE chamber: 10^{-9} Torr to 10^{-11} Torr**
- **On the Moon: approximately 10^{-11} Torr**
- **Interstellar space: approximately 10^{-17} Torr**


NEOCERA
02/01/2008

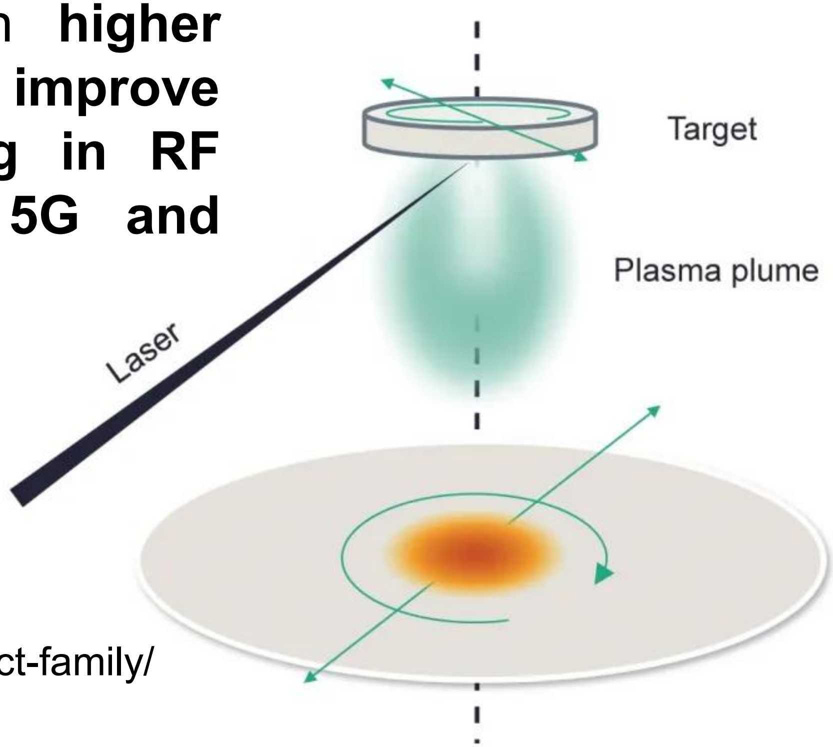


Top Semiconductor Equipment Suppliers



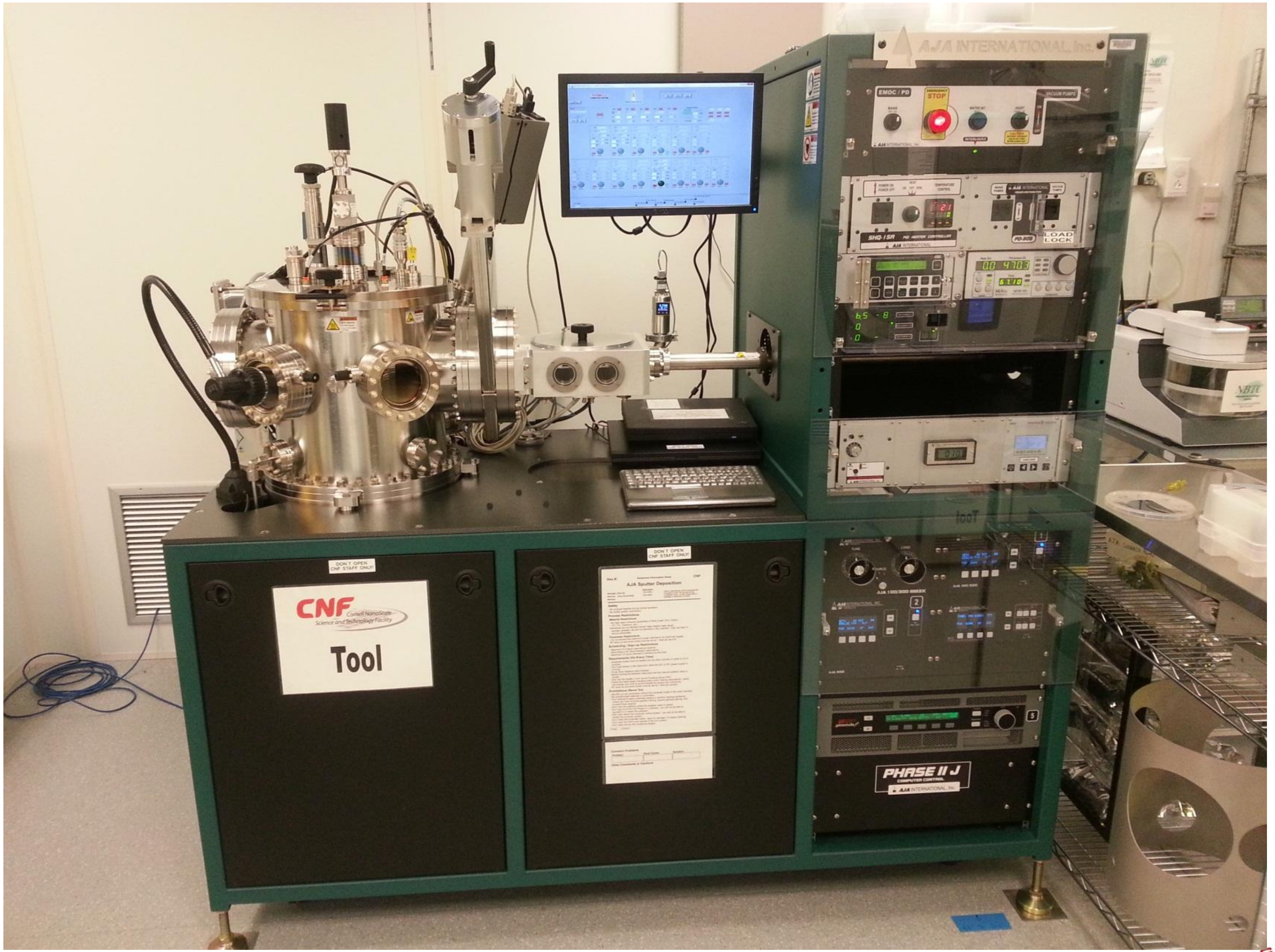
https://www.financecharts.com/sectors/information_technology/semiconductor_equipment#:~:text=TTM%20Total%20Rtn-,Biggest%20Semiconductor%20Equipment%20Companies%20by%20Market%20Cap%202023,and%20Lam%20Research%20(LRCX).

Lam Research is now shipping Pulsus, a production-oriented **pulsed laser deposition (PLD)** tool, to select specialty device manufacturers. **Pulsus PLD** of scandium-doped aluminum nitride films with **higher piezoelectric coefficient will help improve voice control and noise filtering in RF MEMS based microphones for 5G and beyond.** (See figure 3, below)

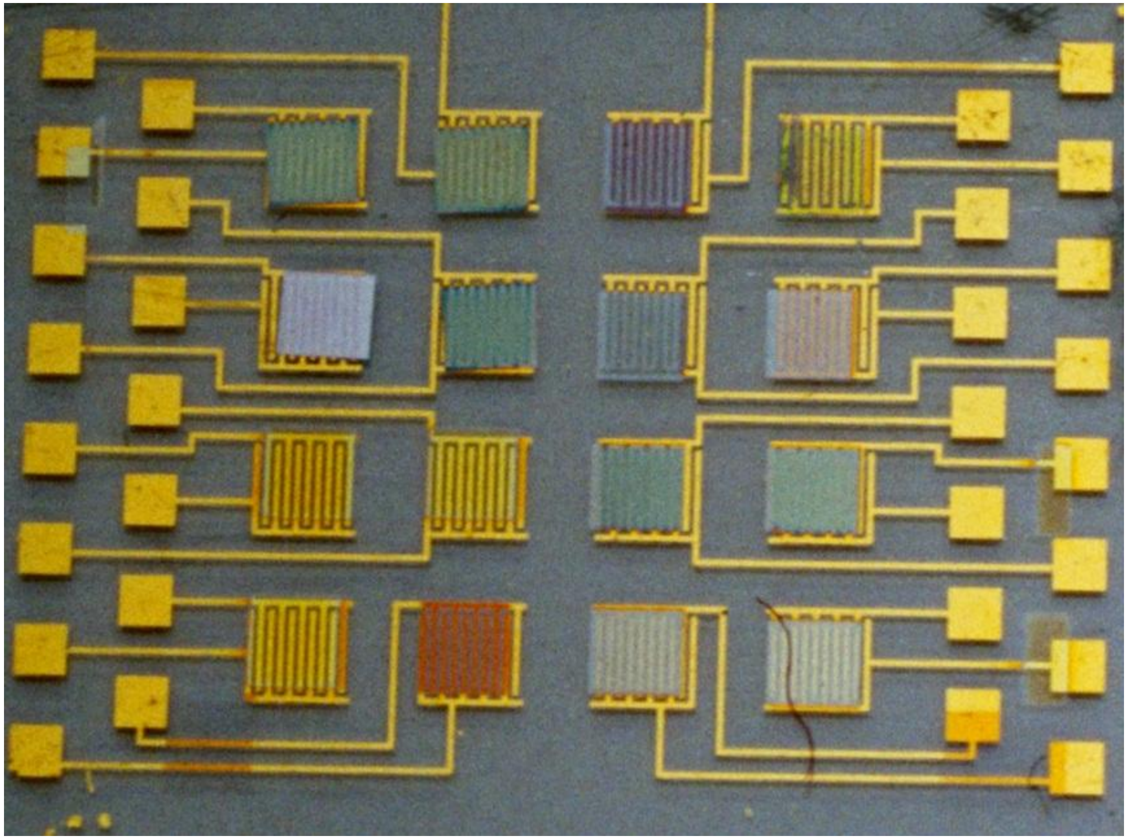


https://www.lamresearch.com/product/pulsus-product-family/

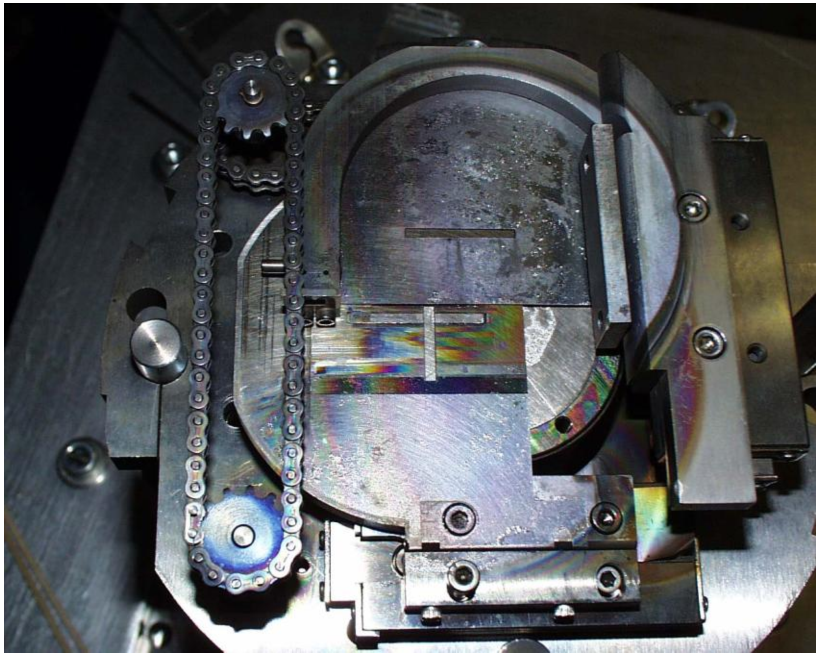
Fig. 2: Pulsed laser deposition process. Source: Lam Research

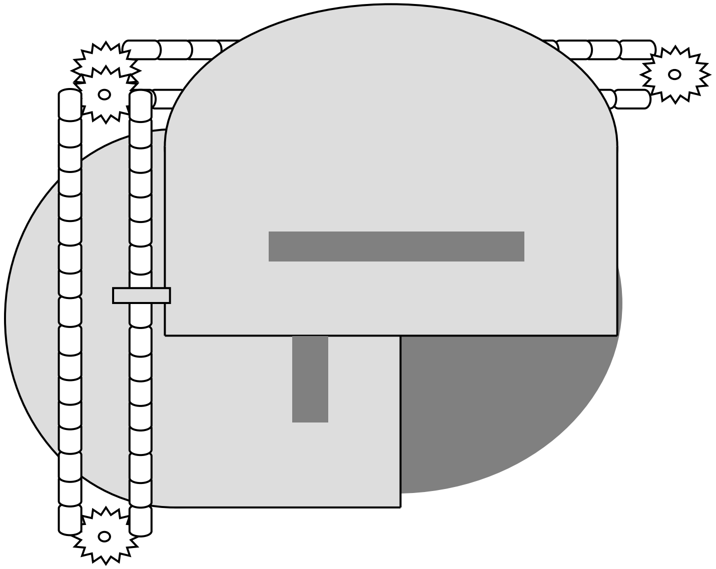

AJA INTERNATIONAL, Inc.
CNF
Tool
PHASE II J
AJA Sputter Deposition
LOAD LOCK

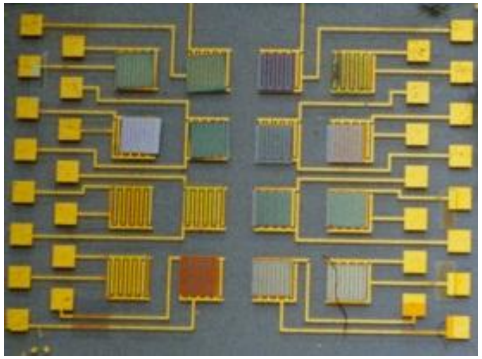
1. Discrete library



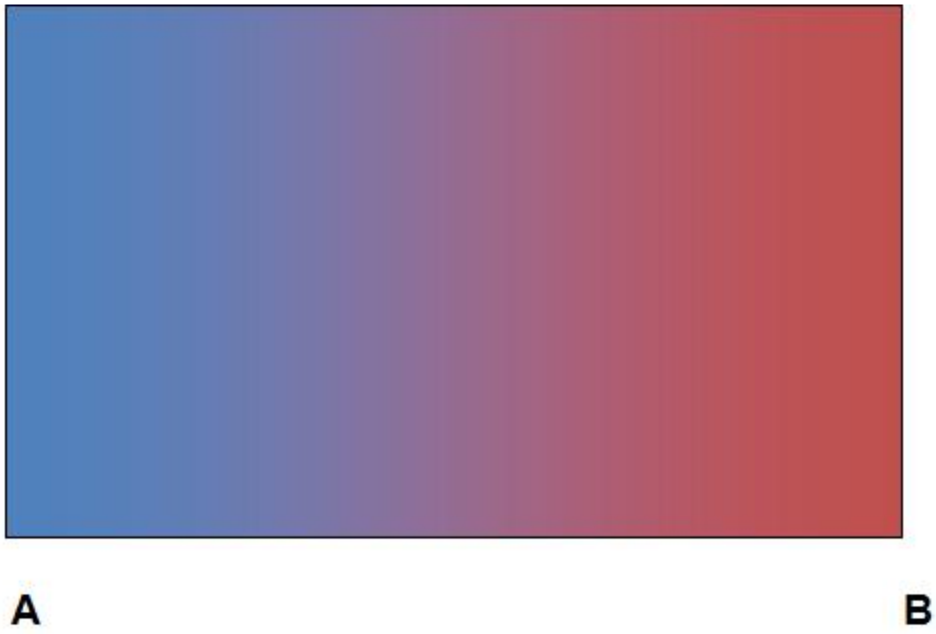
gas sensors

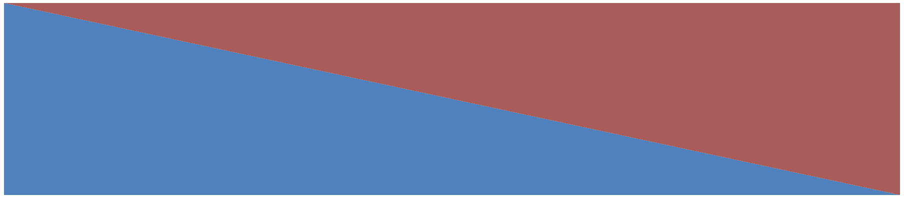


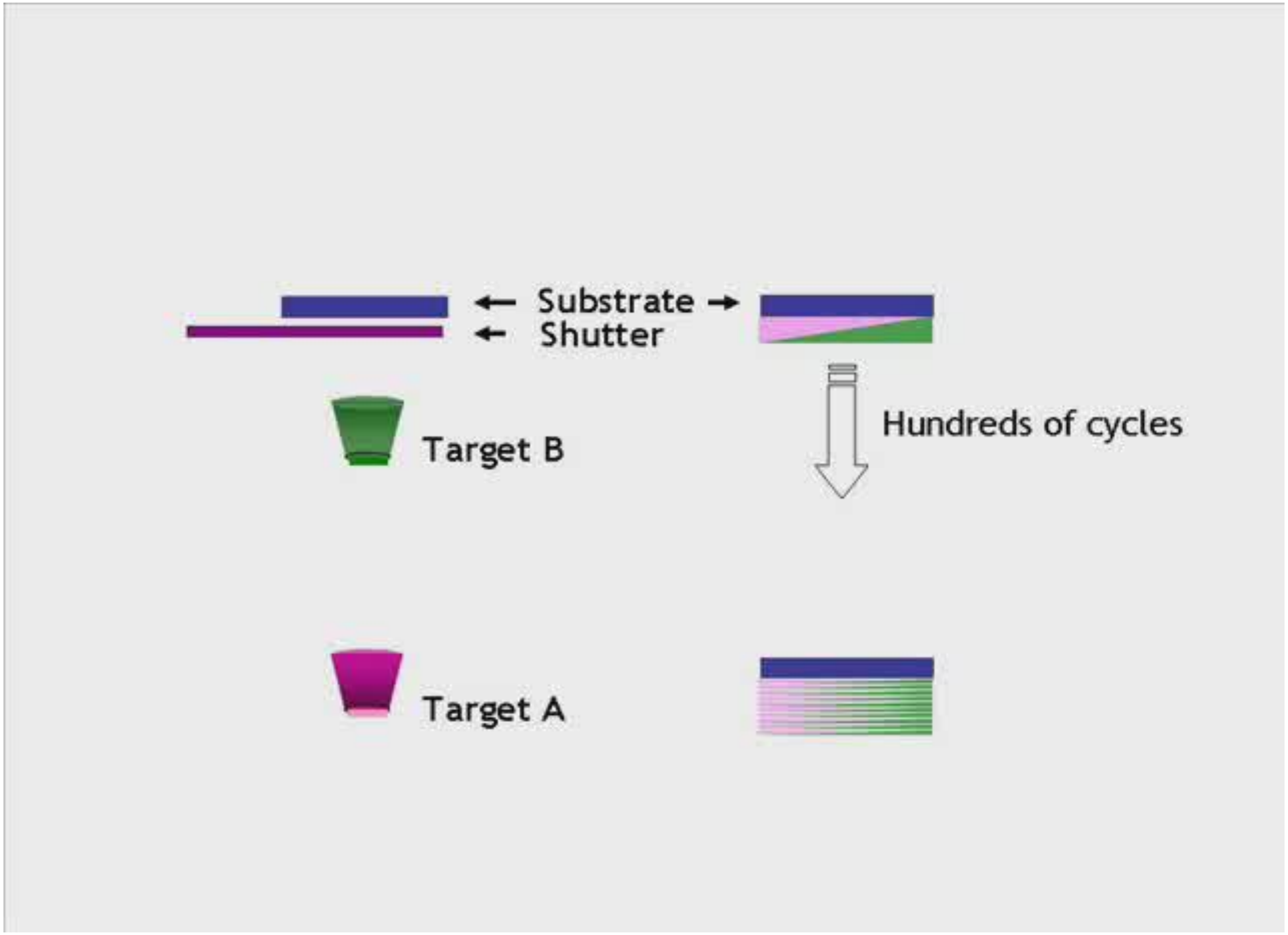




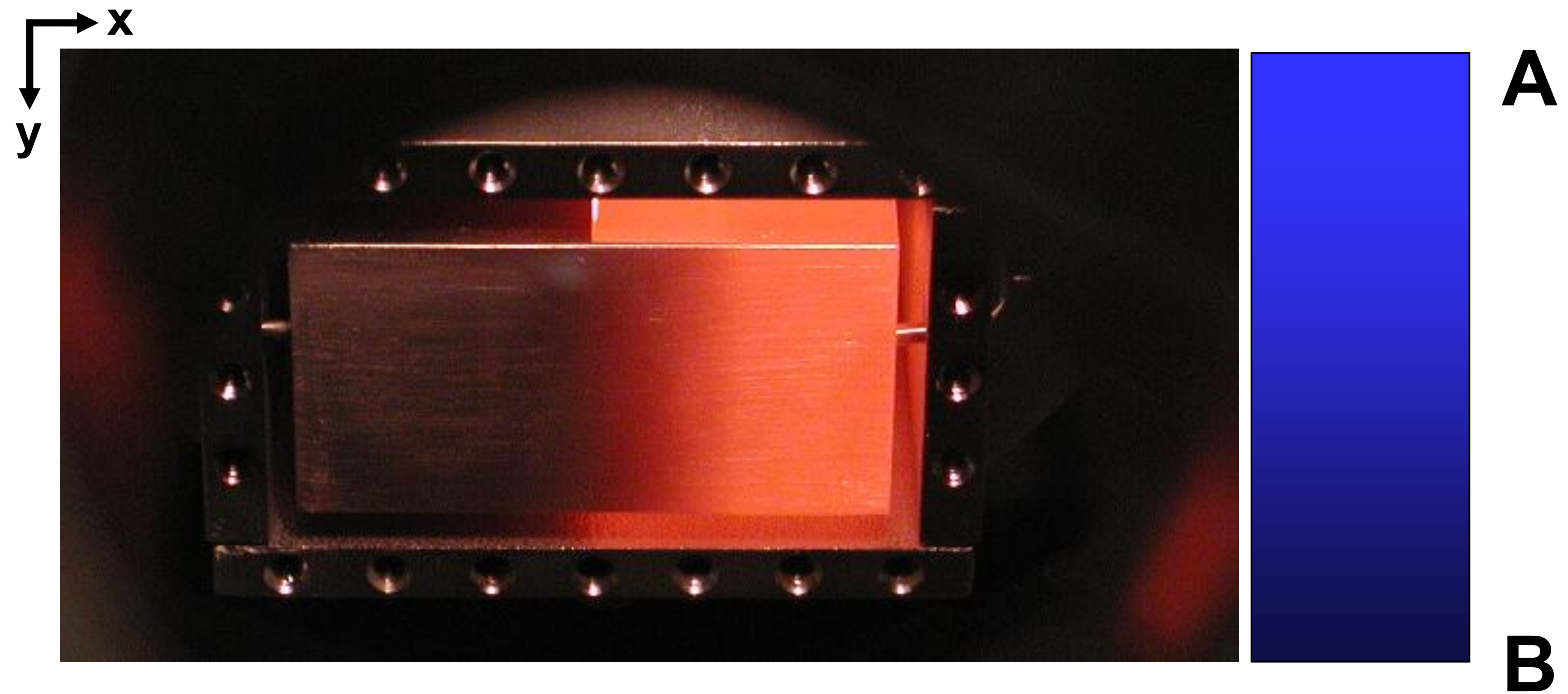
2. Composition spread

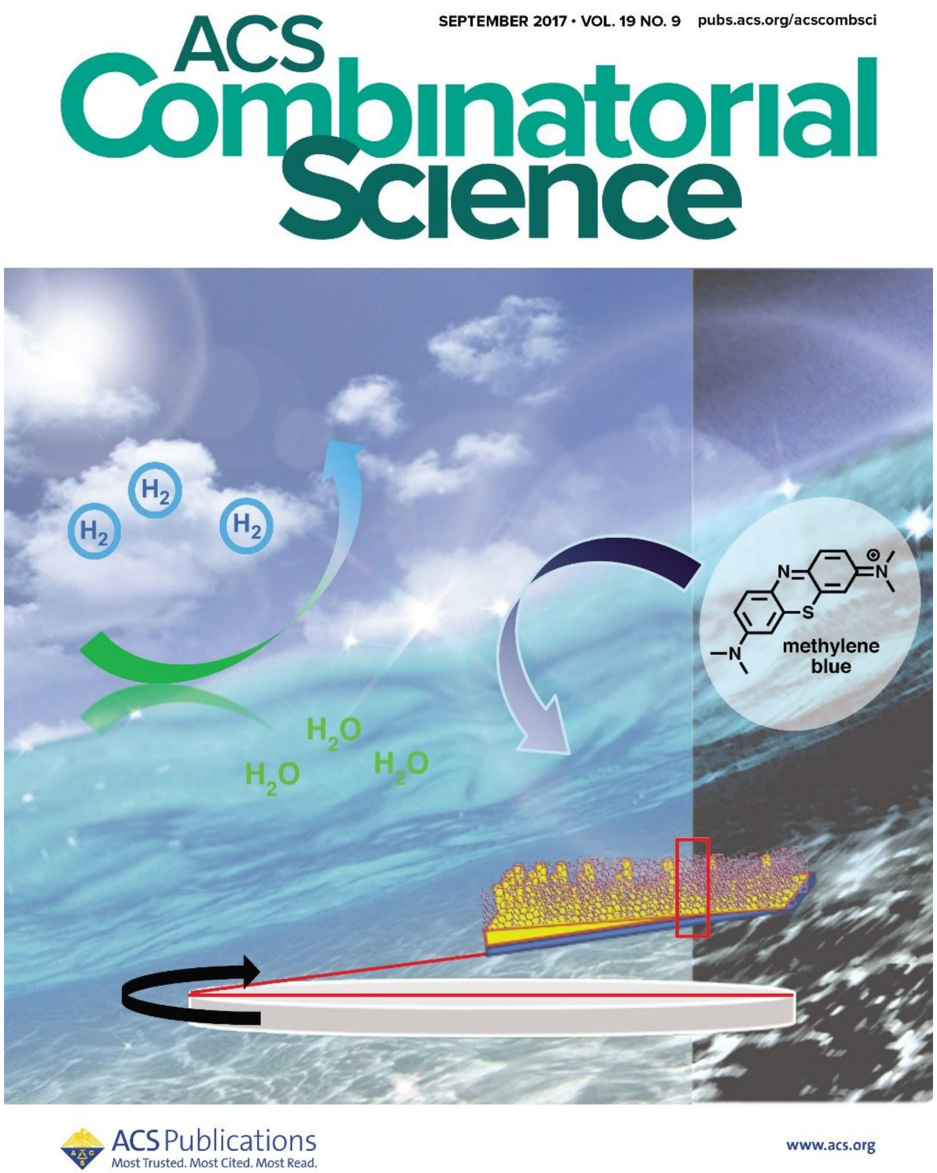





Substrate
Shutter
Target B
Target A
Hundreds of cycles

3. Temp. gradient

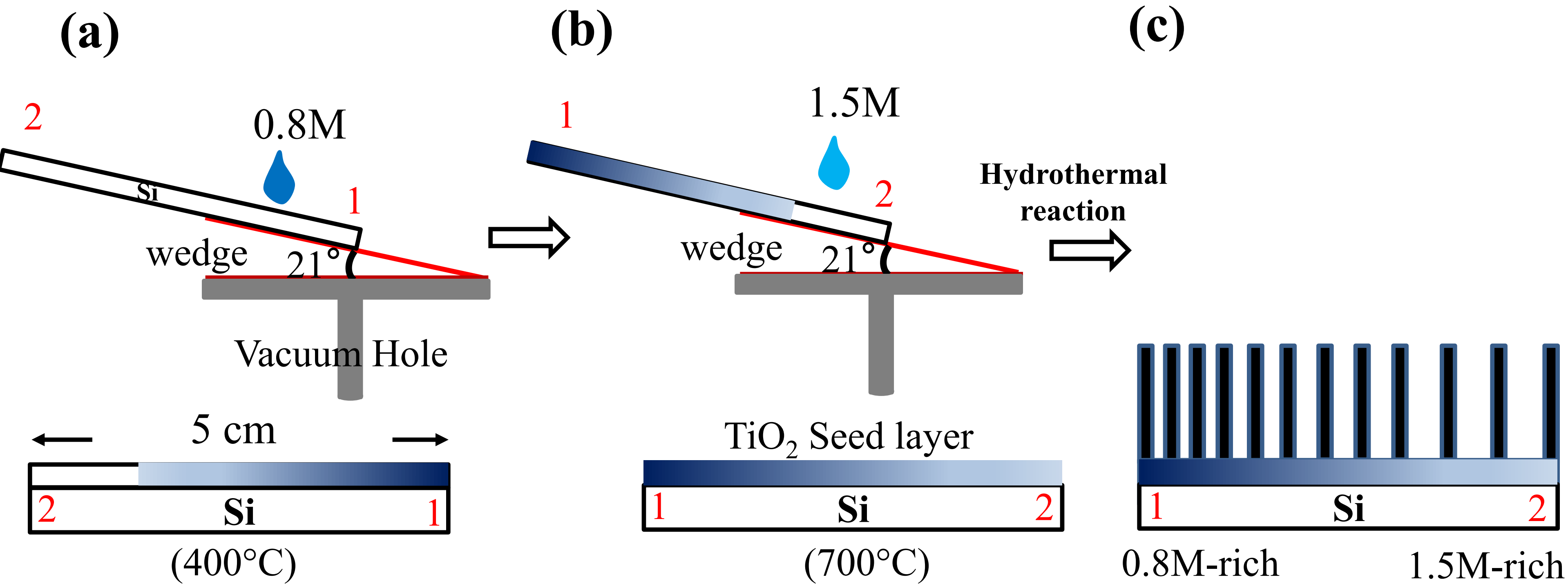




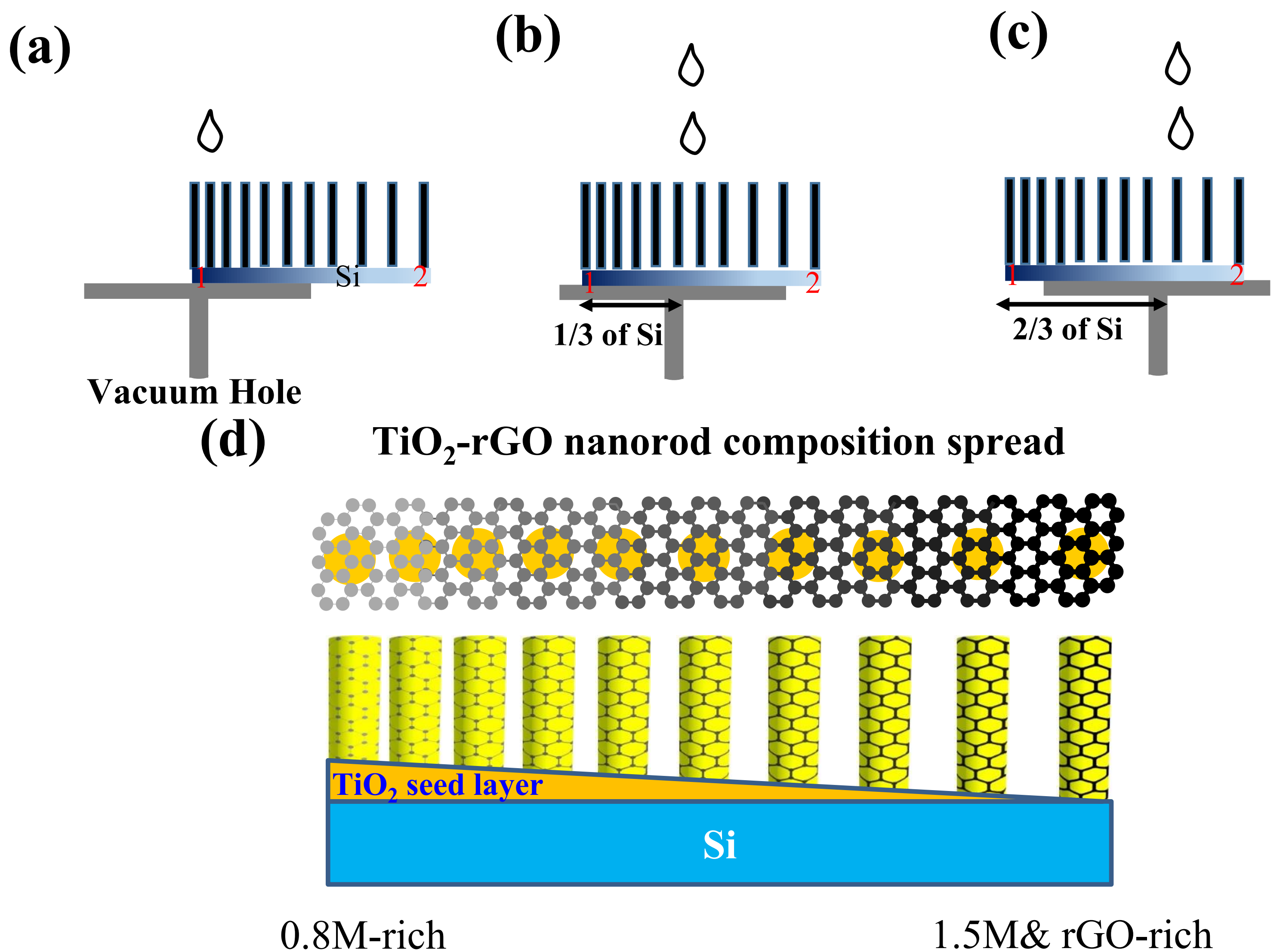
Journal cover story

ACS Combinatorial Science, 19, 585 (2017)

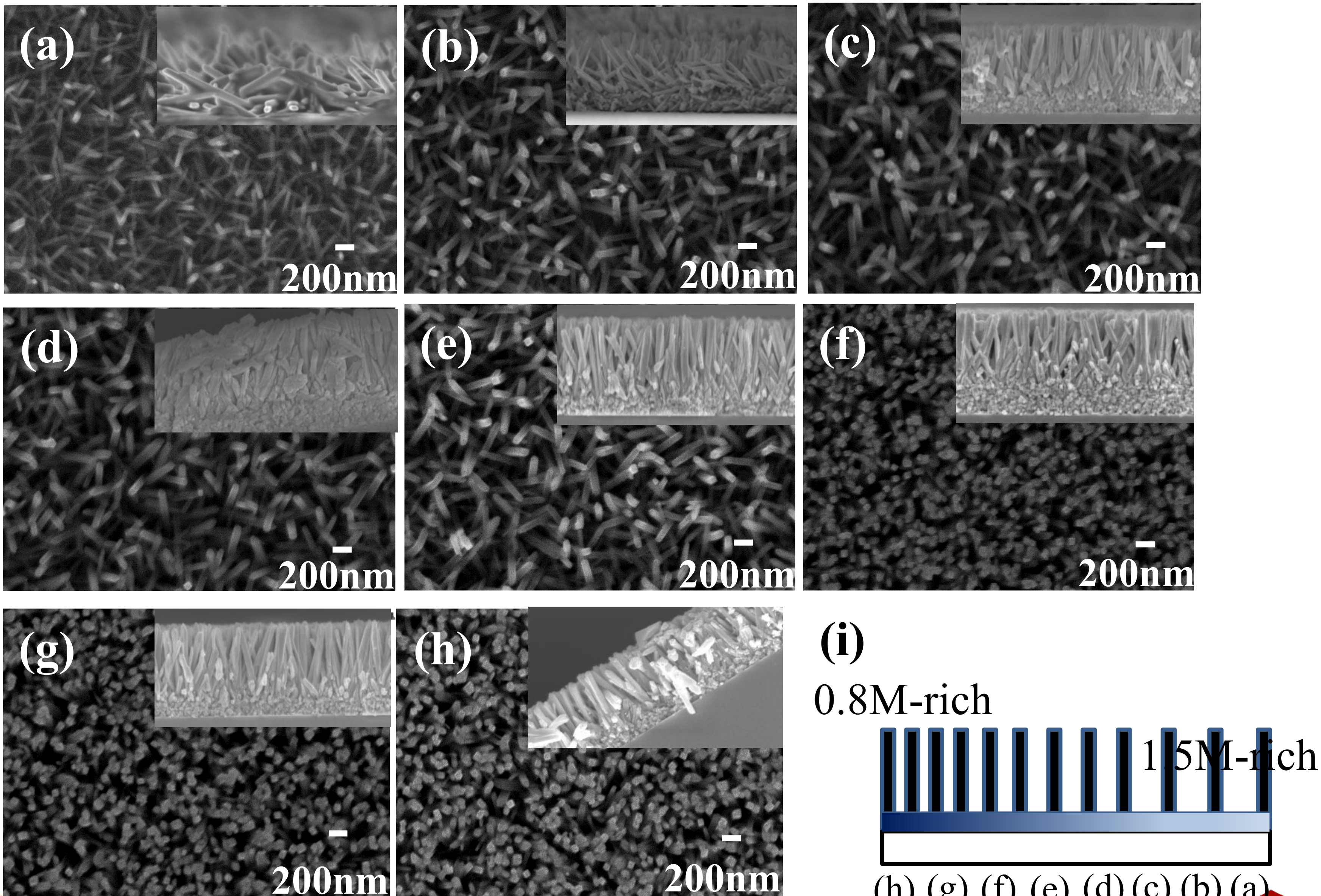
Fabrication of Density Gradient TiO_2 Nanorods



Fabrication of TiO_2–Reduced Graphene Oxide Nanorod Composition Spreads



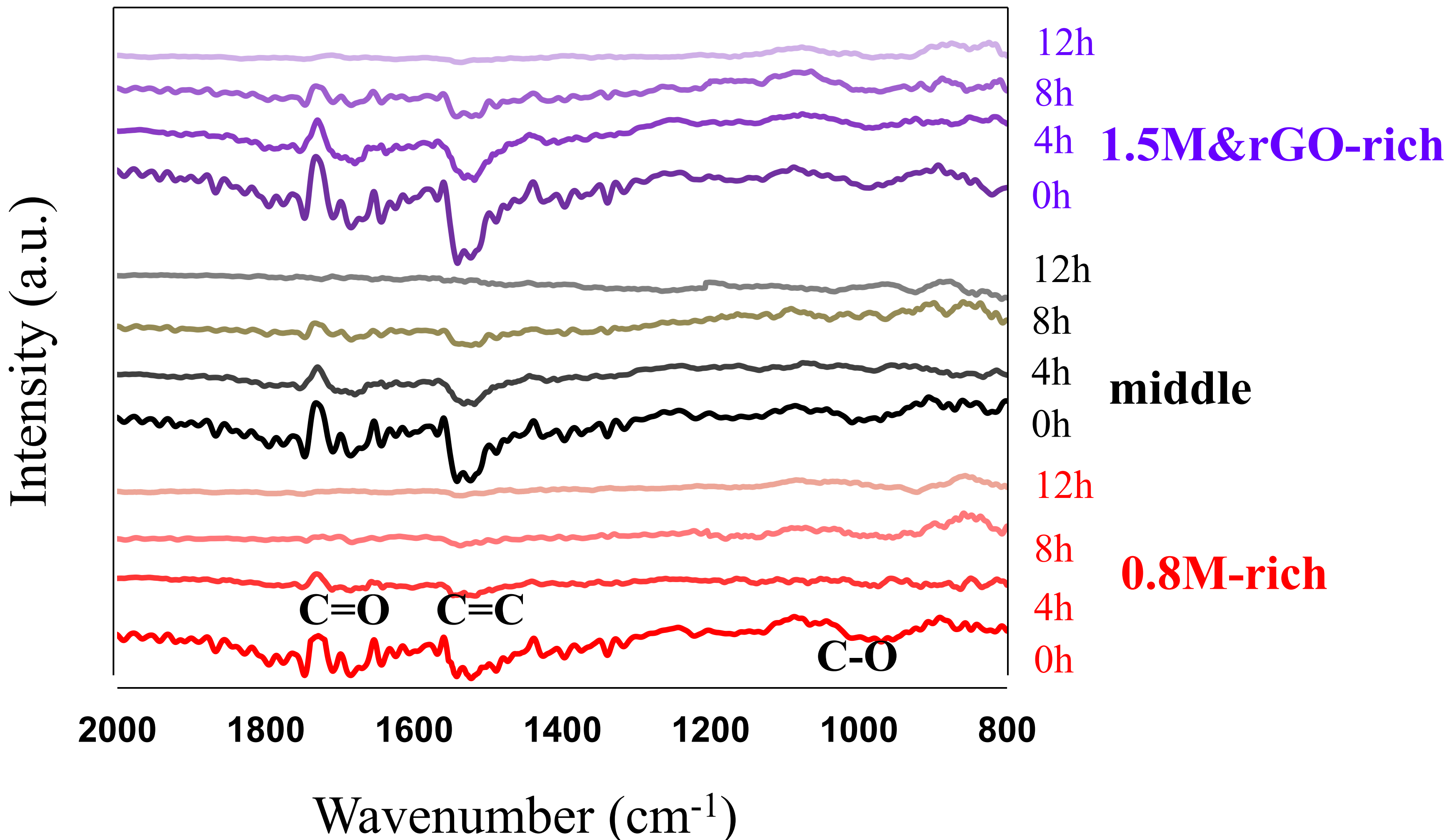
SEM Images of Density Gradient TiO_2 Nanorod Arrays



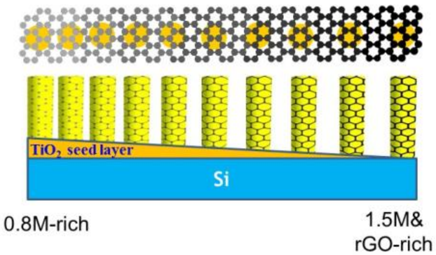
SEM Images of Density Gradient TiO_2 Nanorod Arrays

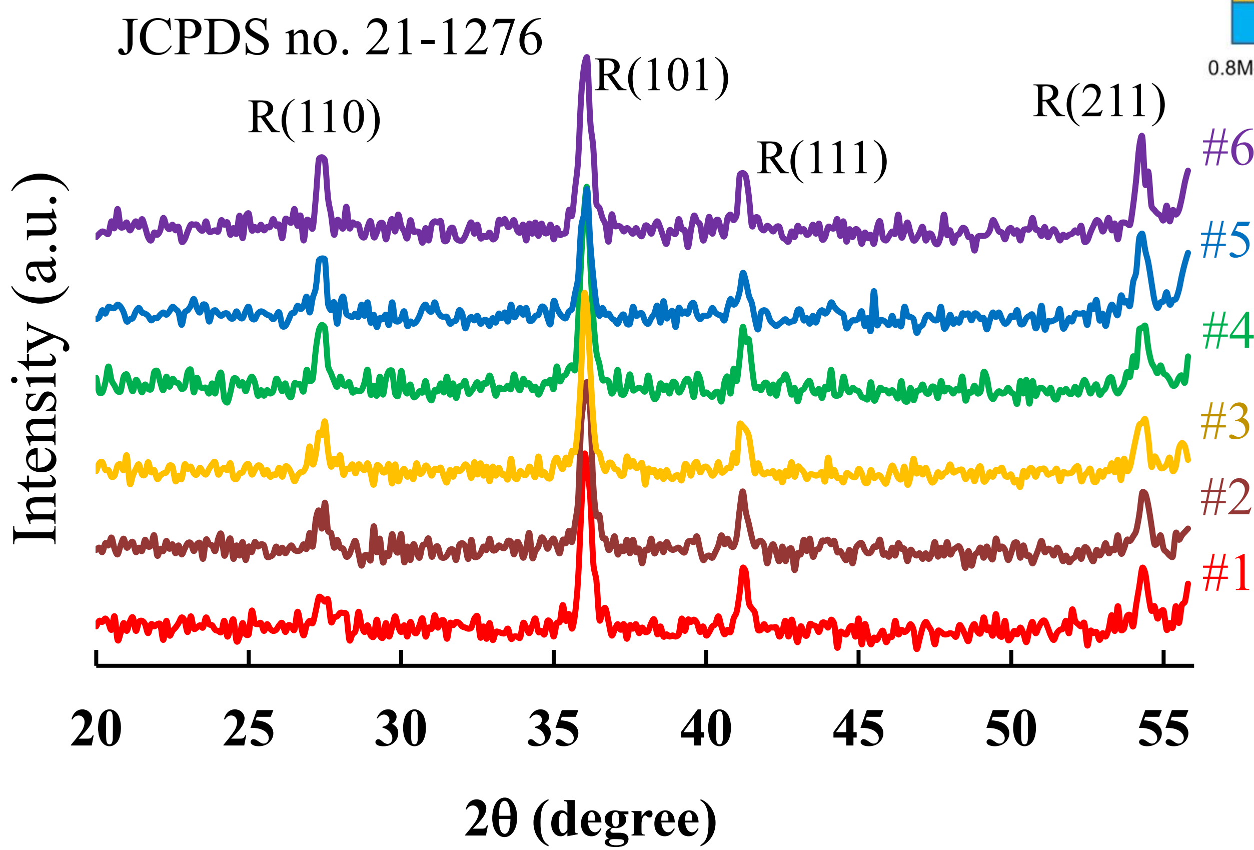
Location	(a)	(b)	(c)	(d)	(e)	(f)	(g)	(h)
# of vertical nanorods (12.5 μm^2)	27	56	70	90	100	500	650	720

FTIR Spectra on TiO_2–rGO Nanorod Composition Spread

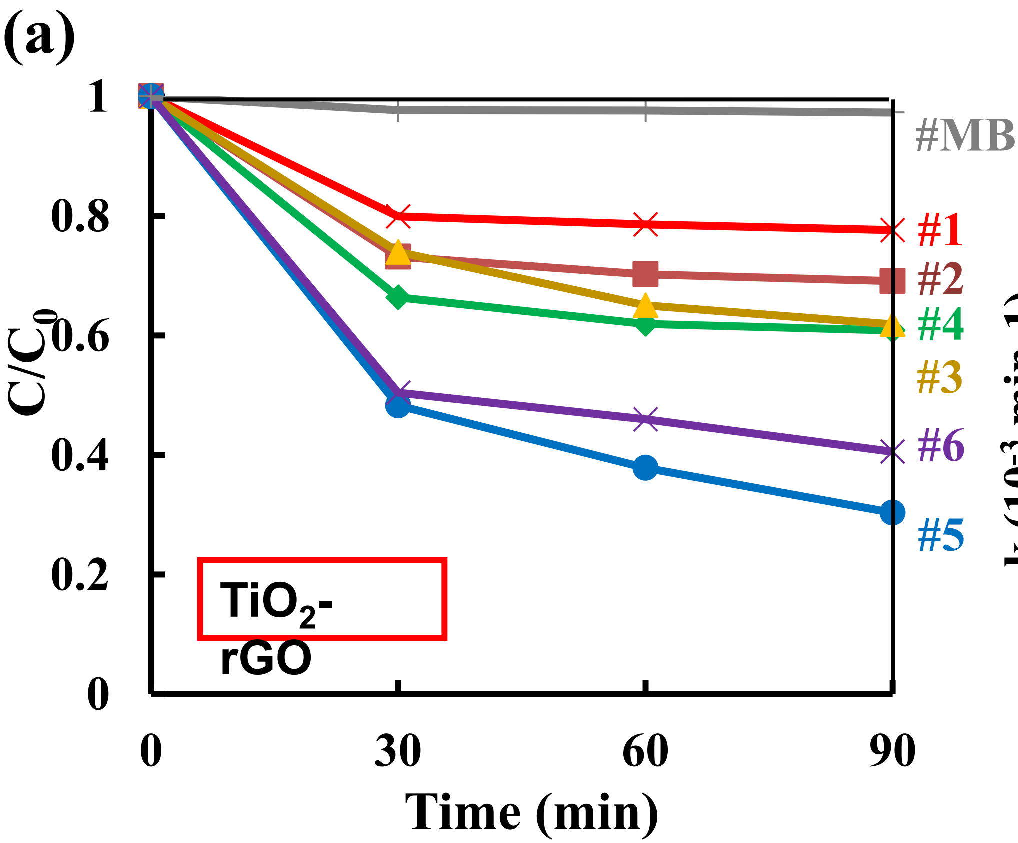


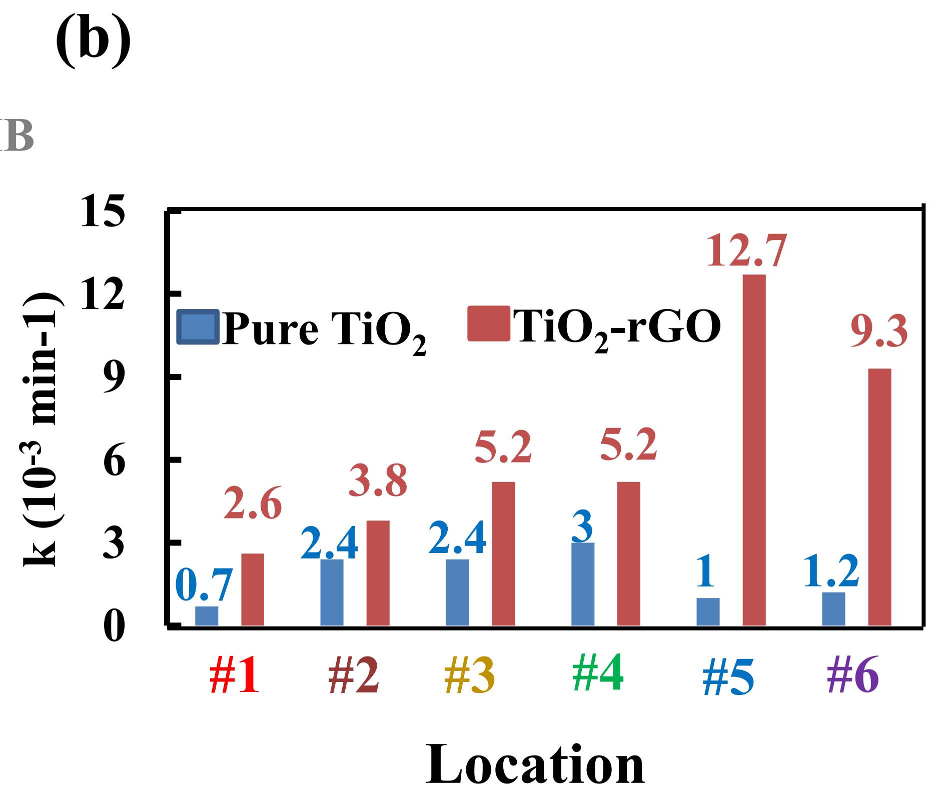
XRD Results on TiO_2–rGO Nanorod Composition Spread



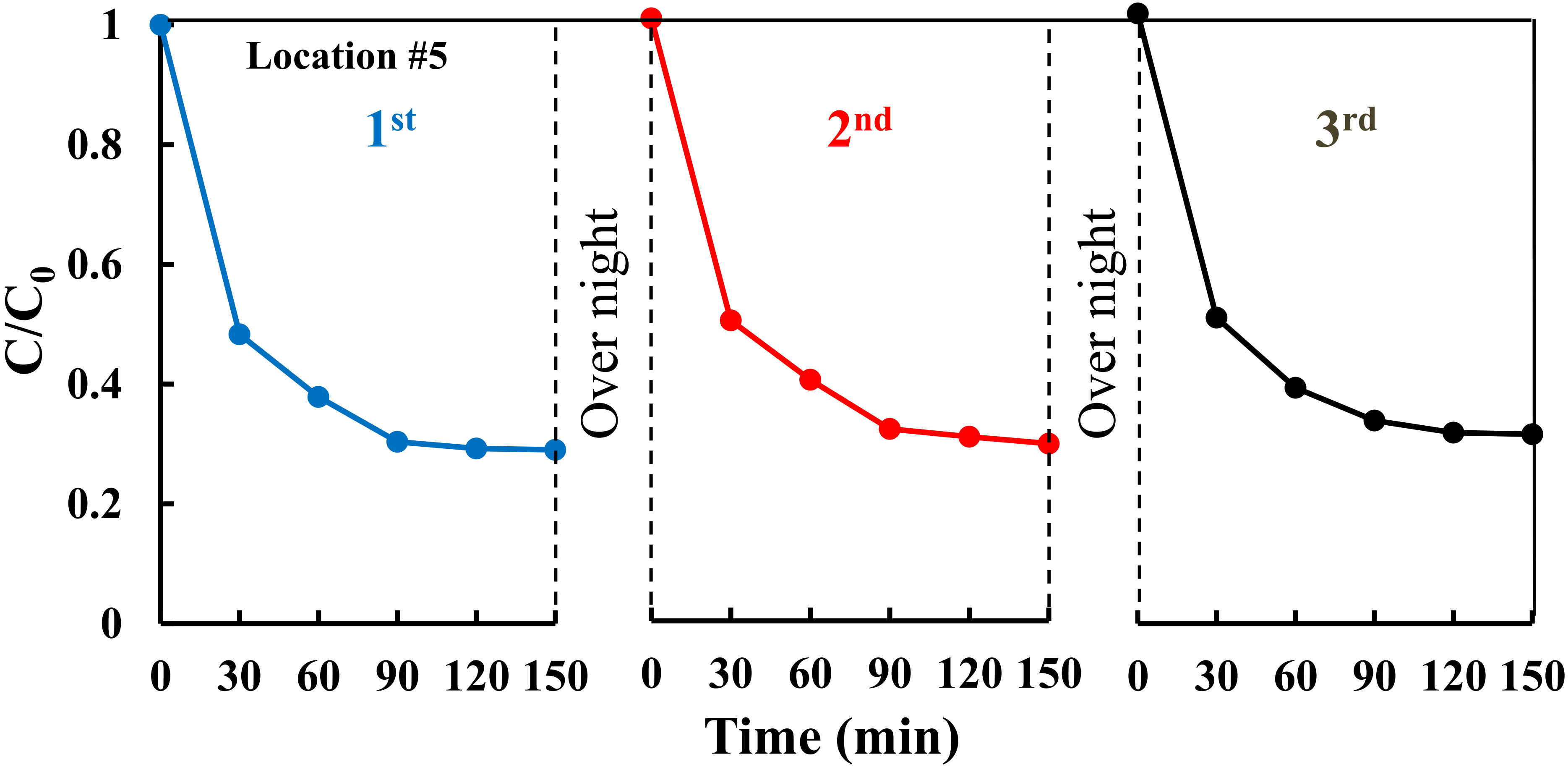


Photodegradation Studies on TiO_2–rGO Nanorod Composition Spread

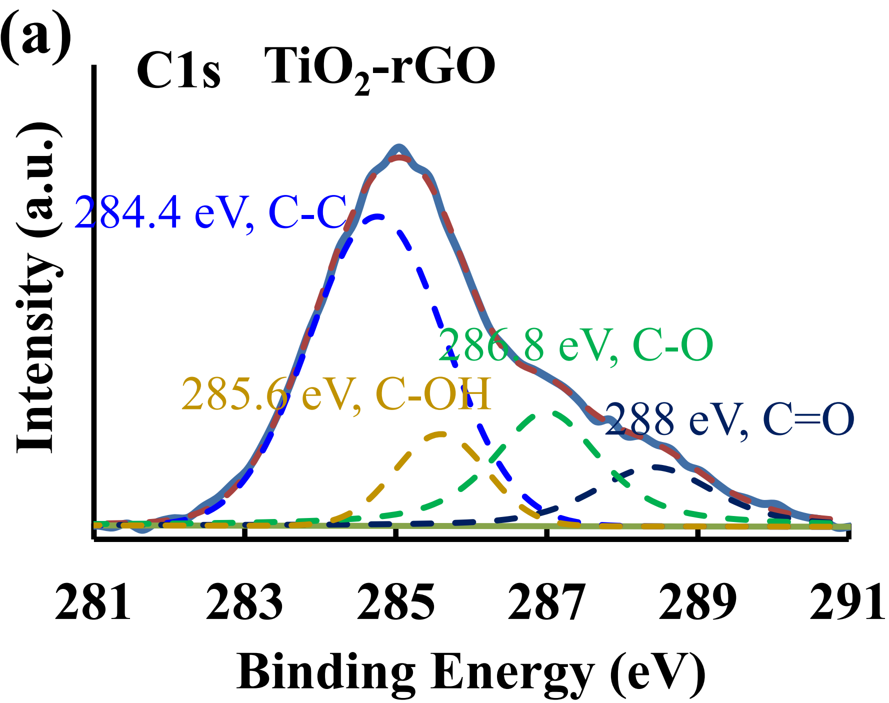


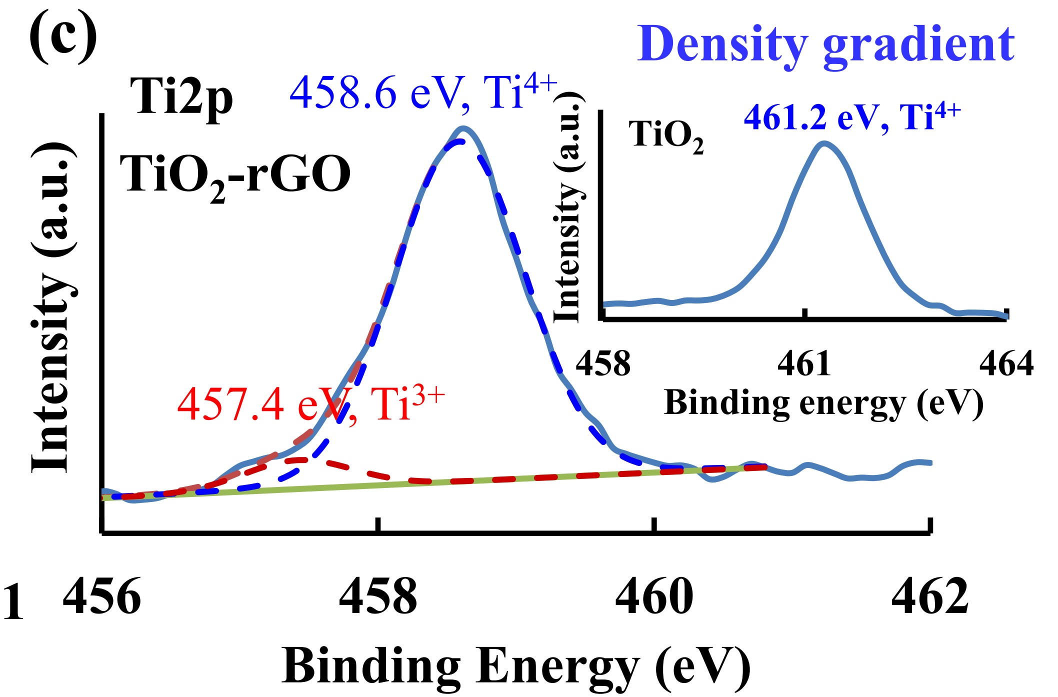


Cycling Test

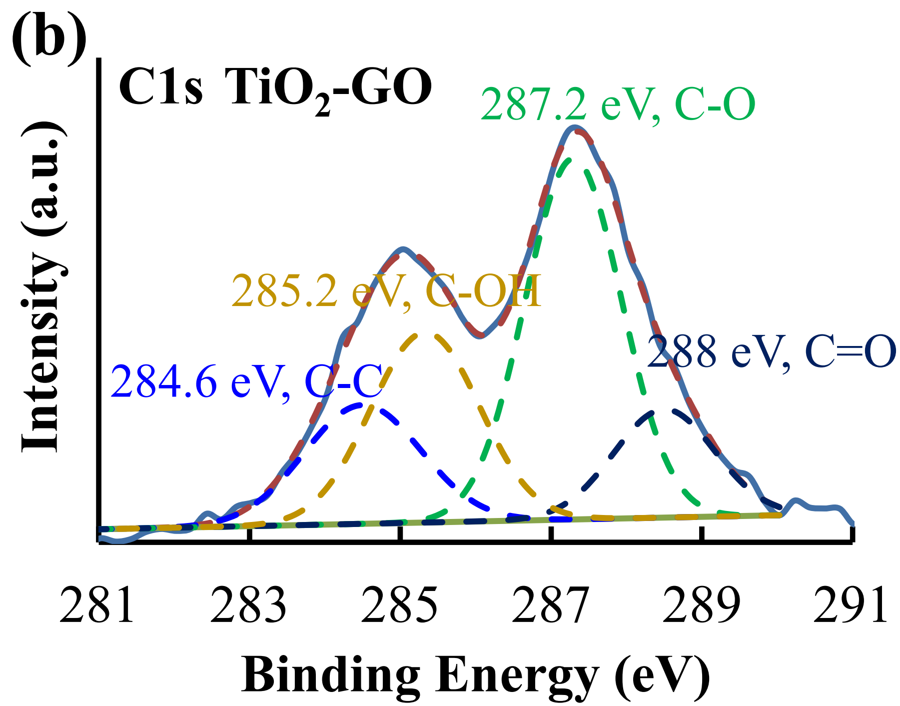


XPS Spectra on TiO_2–rGO Nanorod Composition Spread

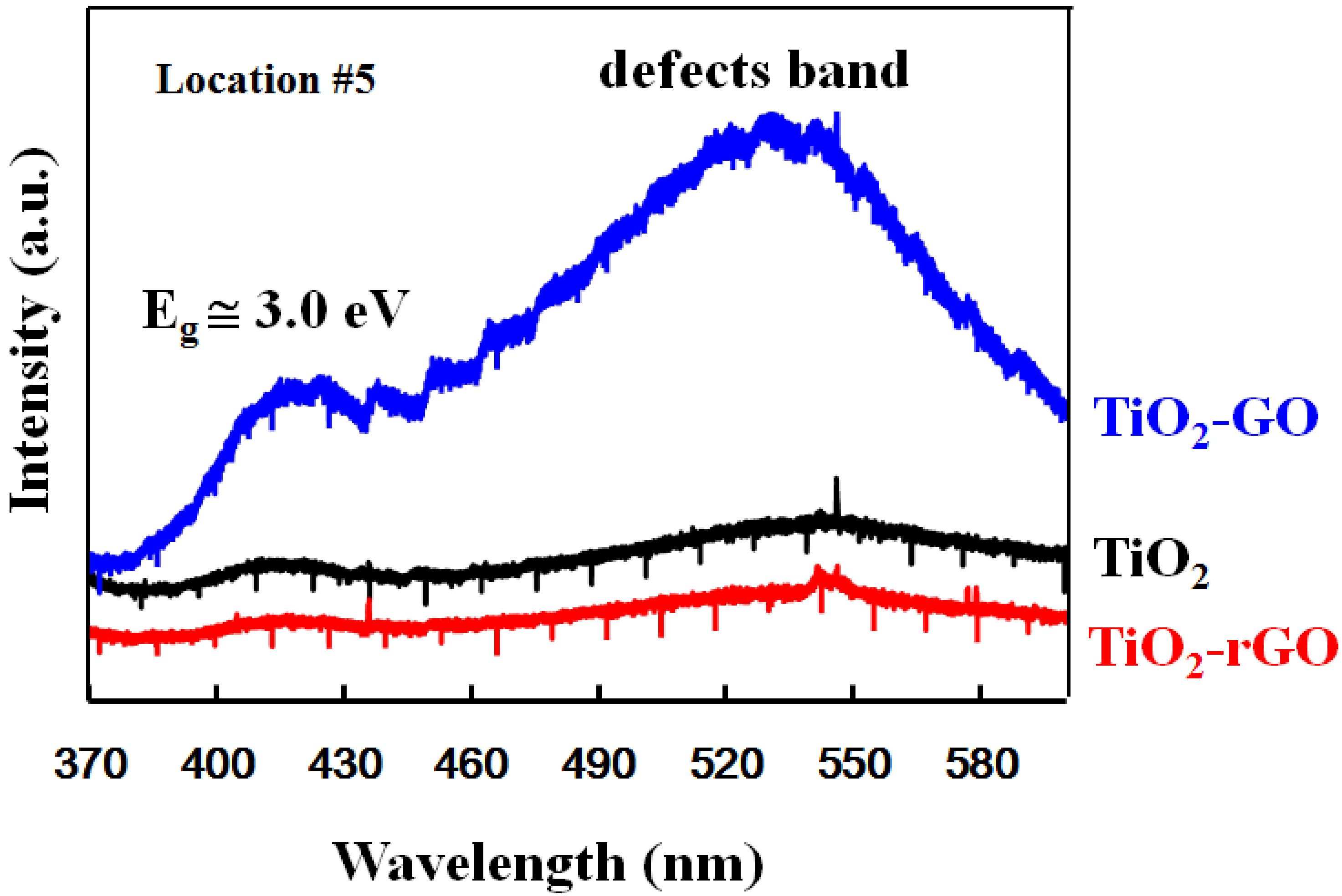




XPS Spectra on TiO_2–GO Nanorod Composition Spread

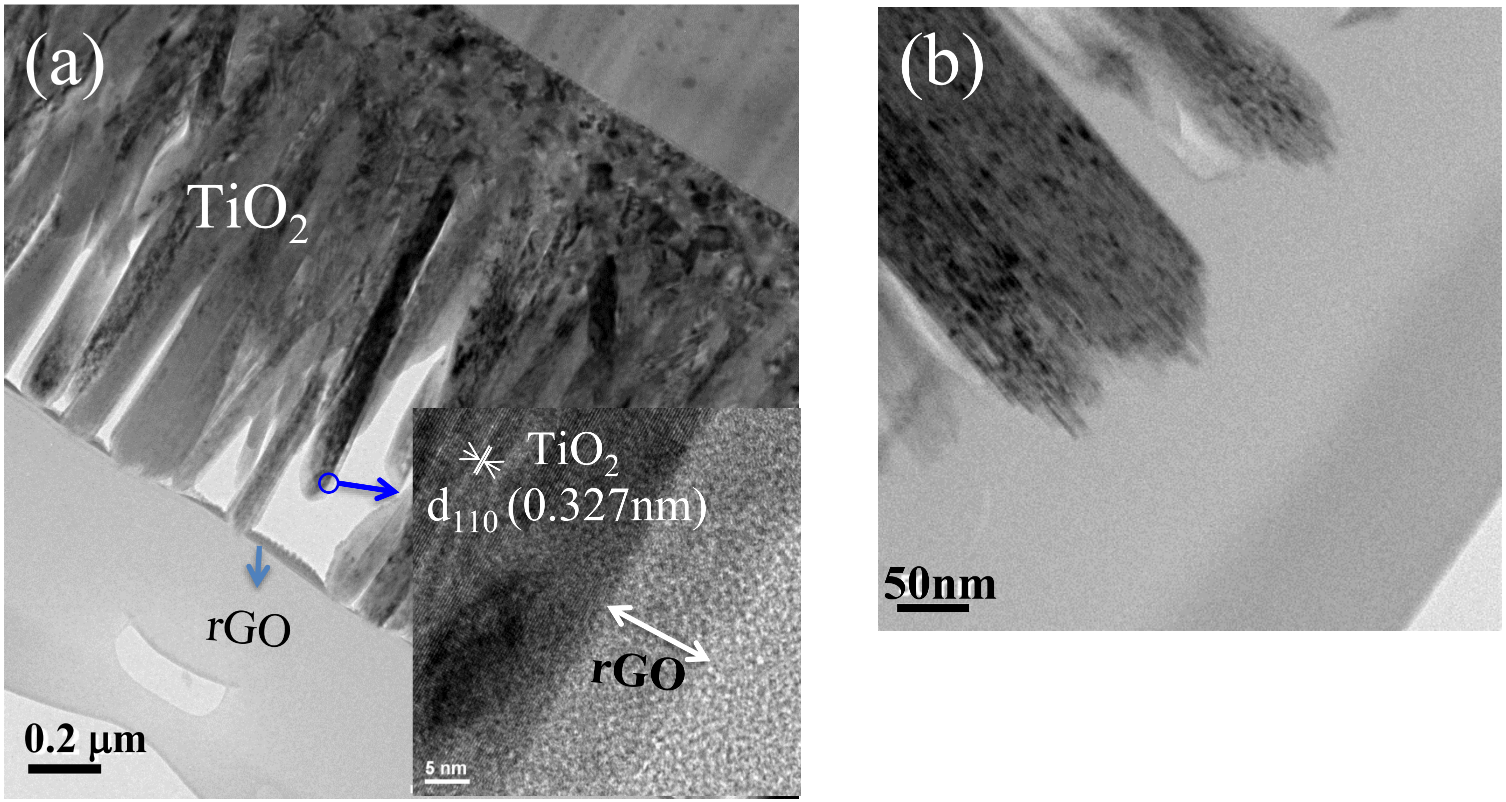


PL Studies

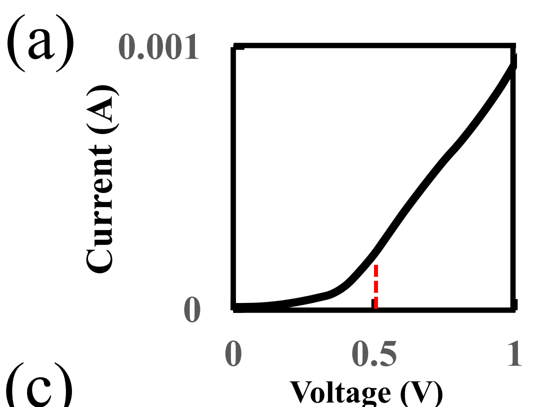


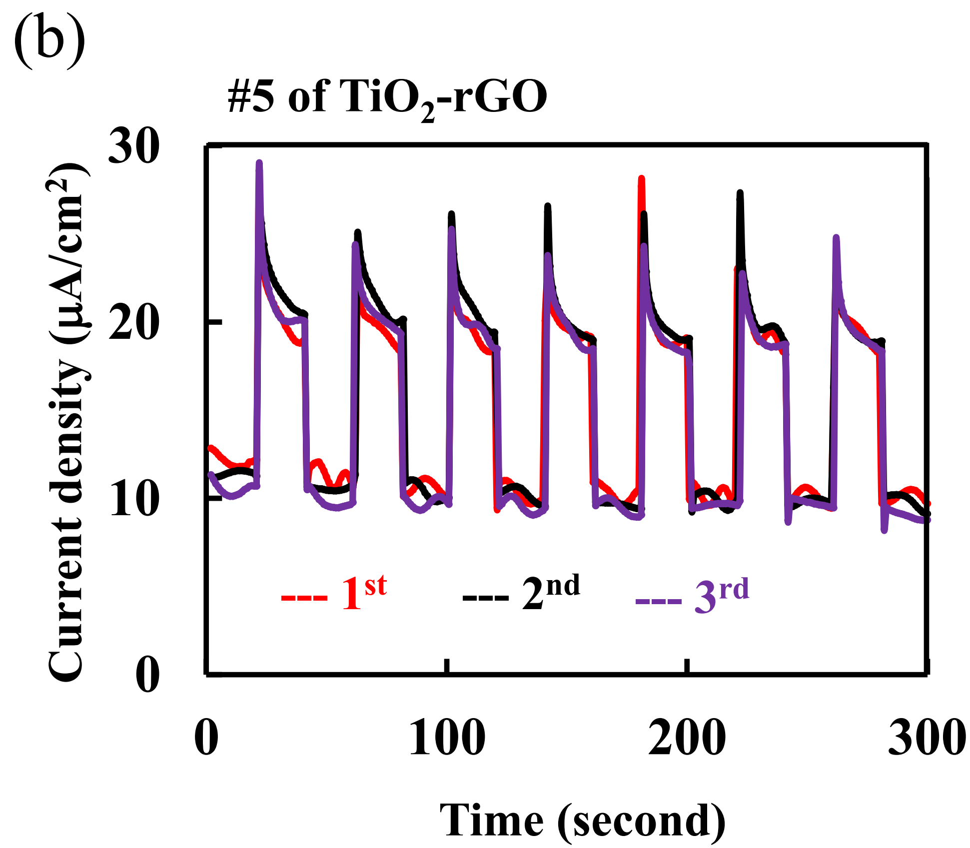
Location #5
defects band
$E_g \cong 3.0$ eV
Intensity (a.u.)
370
400
430
460
490
520
550
580
Wavelength (nm)
TiO_2-GO
TiO_2
TiO_2-rGO

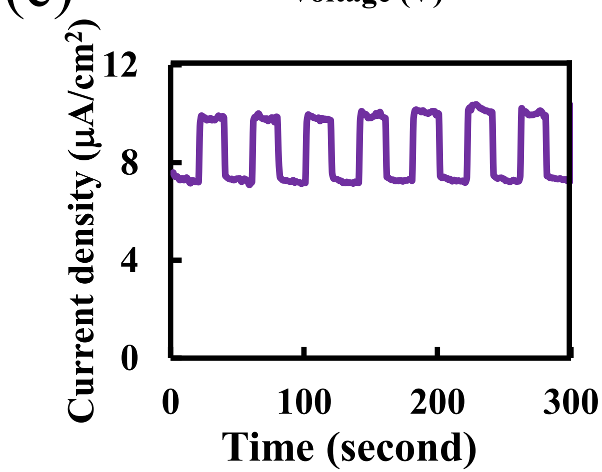
TEM Results



PEC Performance Study







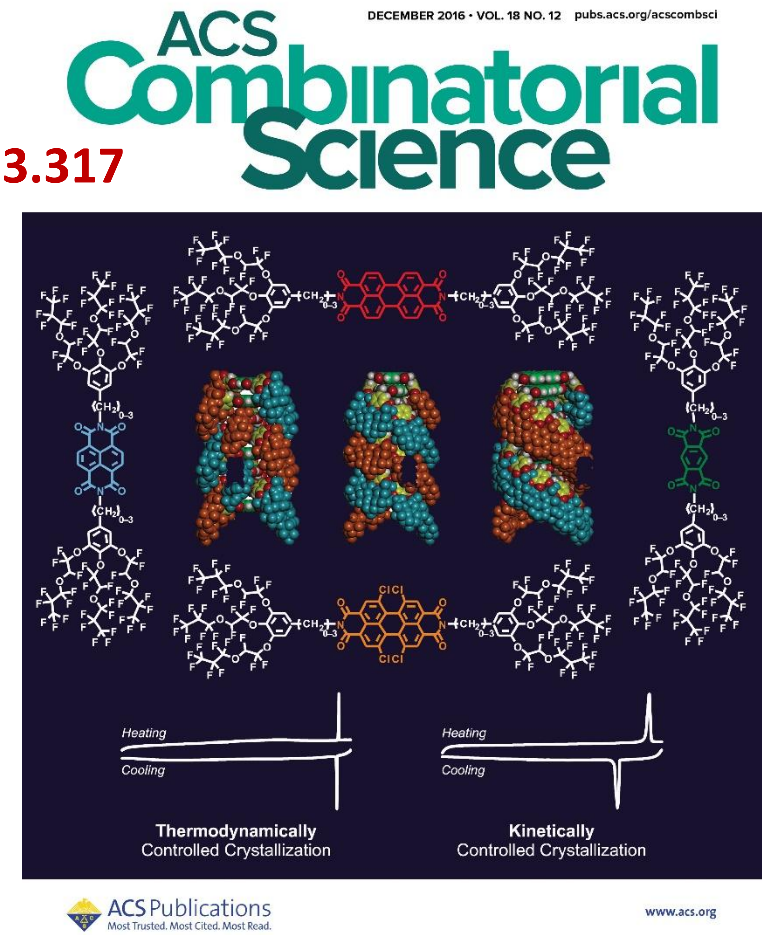
Materials Genome Initiative (MGI)

To help business discover, develop, and deploy new Materials twice as fast, we're launching what we call the Materials Genome Initiative. The invention of silicon circuits and lithium-ion batteries made computers and iPODs and iPads possible – but it took years to get those technologies from the drawing board to the marketplace. **We can do it faster**.

President Obama, June 2011 at Carnegie Mellon University

Combinatorial Journals

IF: 3.317



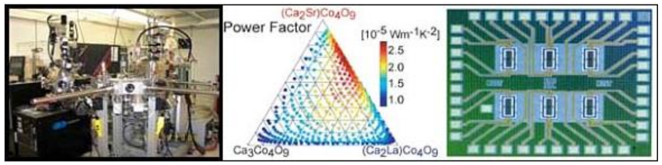
IF: 1.041

JCR Year	CHEMISTRY, APPLIED			CHEMISTRY, MEDICINAL		
	Rank	Quartile	JIF Percentile	Rank	Quartile	JIF Percentile
2015	11/72	Q1	85.417	15/59	Q2	75.424
2014	10/72	Q1	86.806	16/59	Q2	73.729
2013	6/71	Q1	92.254	14/58	Q1	76.724
2012	4/71	Q1	95.070	11/59	Q1	82.203
2011	71/71	Q4	0.704	58/59	Q4	2.542

JCR Year	BIOCHEMICAL RESEARCH METHODS			CHEMISTRY, APPLIED		
	Rank	Quartile	JIF Percentile	Rank	Quartile	JIF Percentile
2015	72/77	Q4	7.143	45/72	Q3	38.194
2014	68/79	Q4	14.557	40/72	Q3	45.139
2013	52/78	Q3	33.974	23/71	Q2	68.310
2012	47/75	Q3	38.000	23/71	Q2	68.310
2011	52/72	Q3	28.472	22/71	Q2	69.718
2010	31/71	Q2	57.042	12/70	Q1	83.571

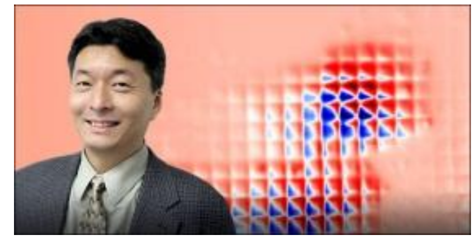
Combinatorial Community

USA



NIST, Dr. Martin Green

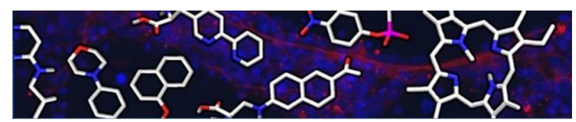
President, Materials Research Society (MRS, 2001)



U. Of Maryland, Prof. Ichiro Takeuchi

Cornell University
Materials Science & Engineering

Prof. Robert Bruce van Dover



Lawrence Berkeley National Lab
Prof. Peter Schultz

Combinatorial Community

USA

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Dr. David S. Ginley

President, Materials Research Society (MRS, 2010)

Dr. John Perkins

Prof. Bruce Parkinson

University of Wyoming

Chemistry & Energy Resources

Prof. Frank Tsui

UNC
COLLEGE OF ARTS & SCIENCES

Combinatorial Community

Japan

THE UNIVERSITY OF TOKYO

Prof. Hideomi Koinuma

National Institute for Materials Science

Dr. Toyohiro Chikyow

U. Of Tokyo
Prof. Masashi Kawasaki

Europe

Dr. Stefan De Gendt

imec

In fiscal year 2012 alone, MGI commitments include:

1. $12 million of research at the **Department of Energy** that will combine computational tools, experimental tools, and digital data to develop and advance high-tech, high-performing materials;
2. $17 million in materials research at the **Department of Defense**, including research to improve the prediction and optimization of materials properties;
3. the launch of **National Science Foundation's** Designing Materials to Revolutionize and Engineer our Future with expected awards to be made in summer 2012; and,
4. efforts at the **National Institute for Standards and Technology (NIST)** to develop new techniques, standards, and tools for the broader research community.

NEW COMMITMENTS by INDUSTRY and UNIVERSITIES

1. **Harvard** to Release 7 Million New Materials Leveraging IBM's World Community Grid and a Partnership with Wolfram Research
2. **31 Companies and Academic Institutions** Make Commitments to the MGI
3. **33 Universities** Pledge to Train Materials Workforce of the Future
4. **ASM International** Launching Center to Accelerate Materials Data Exchange
5. **Autodesk** Releasing Library of 8000+ Materials and Resources to Educate Materials Workforce
6. **Lockheed Martin** Leading New Carbon Nanostructures Consortium
7. **General Electric (GE)** Enhancing Industry-University-Public Interactions

BUILDING ON PROGRESS: BROAD ACTIVITIES BY NATIONAL LABS AND FEDERAL AGENCIES IN SUPPORT OF MGI

1. **Argonne National Lab** Assembling MGI Ecosystem in the Chicago Metropolitan Area
2. **Berkeley National Lab** Tripling Supercomputing Hours for Materials Project
3. **National Nanotechnology Initiative** Contributing to the MGI
4. **DOE** Leads MGI Efforts Across Multiple Programs
5. **NIST** Leads Measurements & Standards Efforts to Support MGI
6. **NSF** Funds Transformative Approaches that Support MGI
7. **DOD** Invests in Research for Materials Innovation Infrastructure

Goals of the Materials Genome Initiative

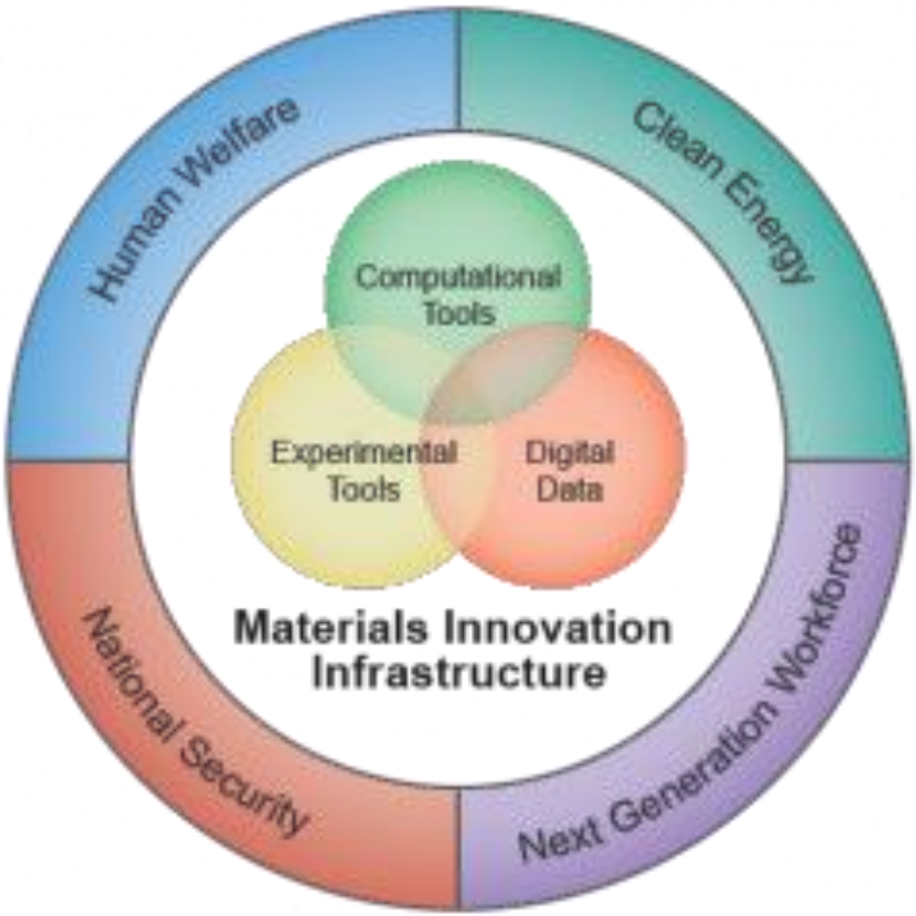
The MGI aims to **double the speed** at which we discover, develop and manufacture new materials by:

- Developing a "**materials innovation infrastructure**" that includes:
  - **Computational tools**: software for predictive modeling, simulation, design and exploration
  - **Experimental tools**: synthesis and processing; quantitative characterization and analytic tools; accelerated testing and rapid prototyping; techniques to validate and advance materials theory
  - **Digital data**: data and interoperability standards for material properties; advanced data mining, analytic tools and open/proprietary data warehouses

Goals of the Materials Genome Initiative

- **Collaborative networks**: integrated centers in computation, data informatics and experimentation; sharing of best practices across disparate centers via formal and informal networking; educational materials for the next generation workforce; public/private partnerships
- Building the materials innovation infrastructure while addressing **high priority material problems of national importance**
- Advancing a culture that supports the use of the materials innovation infrastructure and also embraces a more open, collaborative approach to **developing advanced materials**

Welcome to Materials Genome Initiative (MGI) at NIST



Welcome to Materials Genome Initiative (MGI) at NIST. NIST is working to build the materials innovation infrastructure in support of the Administration's Materials Genome Initiative. Our mission is to accelerate materials innovation with a material genome approach in order to **decrease the cost and time-to-market by 50%.** This site provides the gateway to access all the information on Materials Genome Initiative.

https://mgi.nist.gov/

1. Advanced Composites Pilot for the Materials Genome Initiative
2. ASM Structural Materials Data Demonstration Project
3. Atomistic Potentials and the Future of Nanomaterials Metrology
4. Automation for Atomistic Simulation
5. loud of Reproducible Records
6. Concurrent Experiments and Simulations of Zinc Oxide Nanowires
7. Data and Computational Tools for Advanced Materials Design: Structural Materials Applications - Cobalt Based Superalloys
8. Density Functional Theory (DFT) Informatics and Repositories
9. DFT Benchmarking
10. Directed Self Assembly of Block Copolymers for Nanopatterning
11. Facilitating the Development of Modular Data Models in Materials Science
12. FiPy (an open software framework)
13. Fundamentals of Macromolecular Self Assembly: particles, gels, and polyelectrolyte complex coacervates
14. Generic Materials Design Toolkit
15. Genomics of Electronic Materials **(James C. Booth)**
16. High-Precision Structural Measurements **(Igor Levin)**

17. High-Throughput (Combinatorial) "Foundry" for Inorganic Materials: "Data on Demand" **(Martin L. Green)**
18. High-Throughput Experimental Materials Science Virtual Laboratory **(Martin L. Green)**
19. Integrated Data Management for Materials Discovery
20. Integrated Nanoscale Experimentation, Prediction, and Validation **(Eric Cockayne)**
21. Investigating the Diameter-Dependence of Elastic Moduli of Zinc Oxide Nanowires using Molecular Dynamics Simulations JARVIS-FF
22. Machine Learning for High Throughput Materials Discovery and Optimization Applications **(Martin L. Green)**
23. Materials Data Curation System
24. Materials Data Repository
25. Materials Informatics
26. Materials Resource Registry
27. MGI Code Catalog
28. Modeling Dispersion Rheology for Non-Spherical Particles
29. Multiscale MD-FEM Methodology
30. NIST Center for Automotive Lightweighting (NCAL)
31. NIST/MML Center for Theoretical and Computational Materials Science
32. Object Oriented Finite Elements (OOF)
33. OpenCALPHAD

34. Searching the ICSD for new functional materials from first principles
35. Semi-Automatic Curation
36. Strategy for extensible, evolving terminology for MGI efforts
37. Structure-Property Links in Deformation of Materials
38. Transport Properties of Complex Particles and Polymers
39. Uncertainty Quantification in Computational Materials Science
40. Validation of Classical Atomistic Simulations of Nanoscale Material Phenomena
41. Validation of Density Functional Theory for Materials
42. Web Force-Field (WebFF)
43. μMAG: Micromagnetic Modeling Activity Group