SAND2012-3421C
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Research at Sandia National Laboratories:

Enabling the Mission and

Advancing the Frontiers of Science & Engineering

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Deputy Chief Technology Officer

April 26, 2012

Sandia National Laboratories

Exceptional service in the national interest

U.S. DEPARTMENT OF ENERGY

NNSA

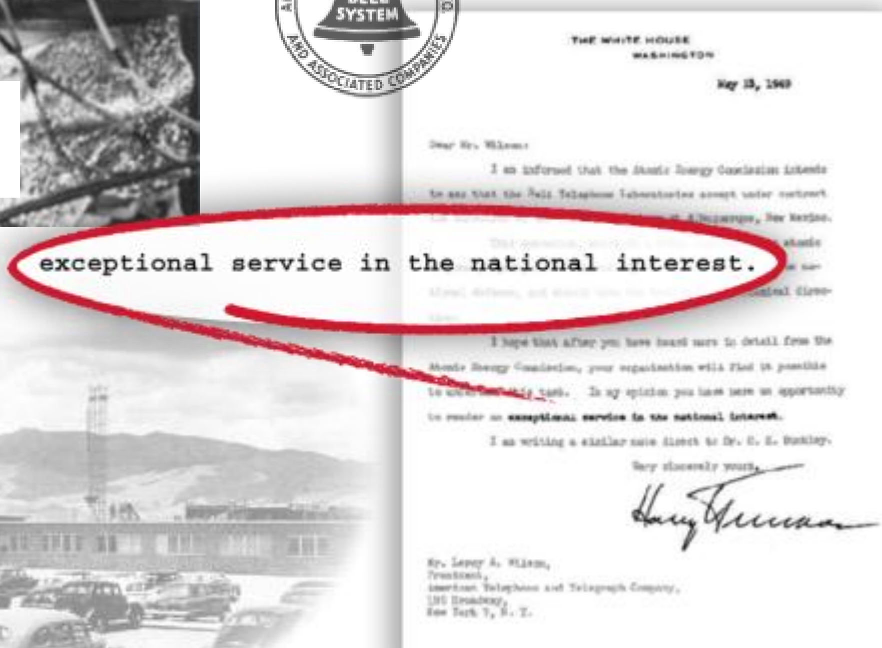
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Outline

- Overview
  - A quick tour of Sandia National Laboratories
  - Sandia's Research Foundations
- Examples of enabling the mission and advancing the frontiers of science and engineering

Sandia has served the nation since 1949

Jerrold Zacharias, c1945,
led the transfer of the Z Division
to SNL from LANL



Sandia's Sites

Livermore, California

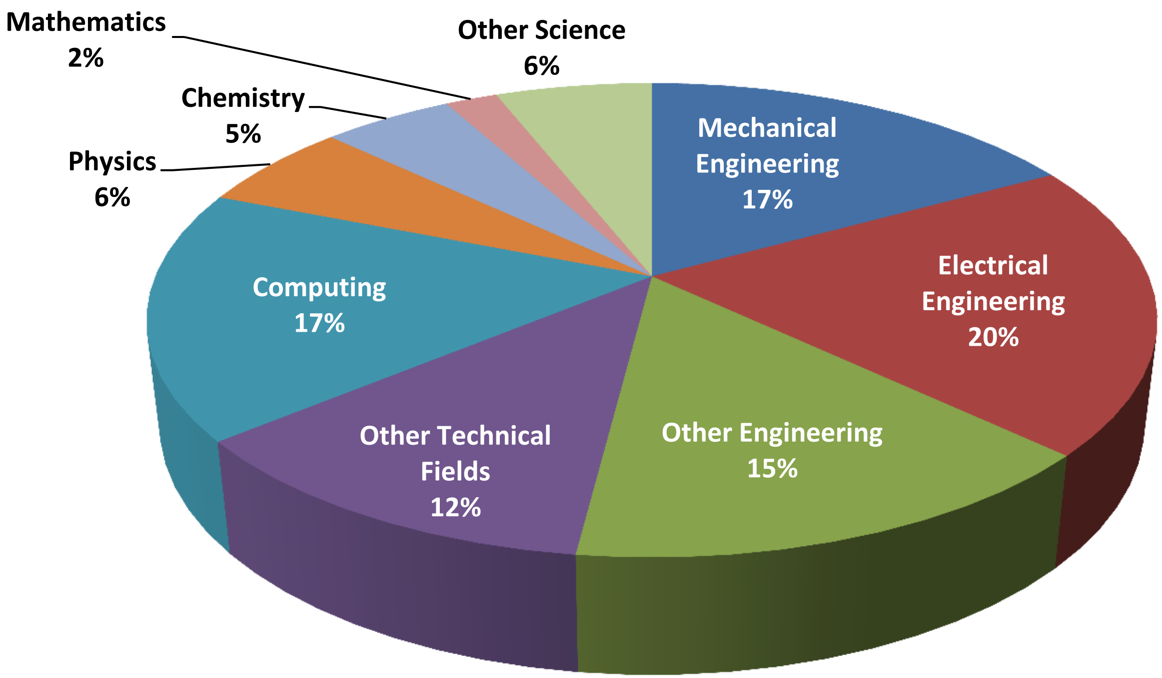
Albuquerque, New Mexico

Tonopah, Nevada

Waste Isolation Pilot Plant, Carlsbad, New Mexico

Pantex, Texas

Sandia's Workforce



UNM Alumni

PhDs	Masters	Bachelors
144	787	494

- **On-site workforce: 10,459**
- **Regular employees: 8,949**
- **Technical Staff: 4,357**

Mission: National Security

Nuclear Weapons

Energy Climate and
Infrastructure Security

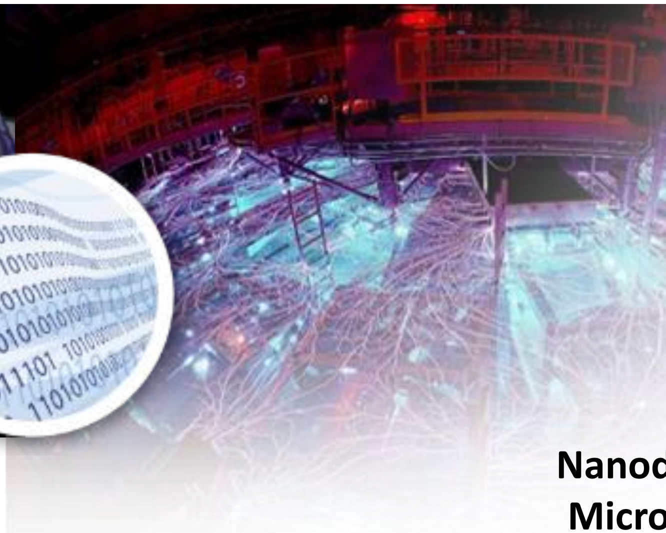
International Homeland and
Nuclear Security

Defense Systems
and Assessments

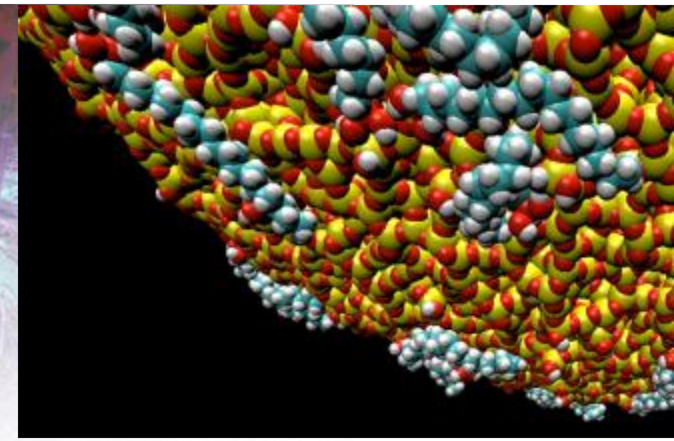
Strong Research Foundations Enable Mission Performance

Computing & Information Sciences

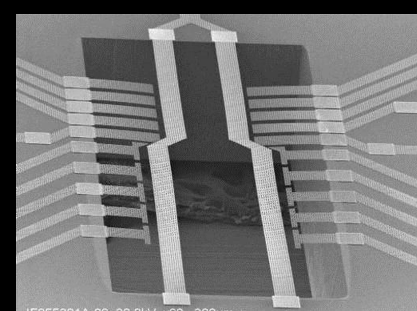
Radiation Effects & High Energy Density Science



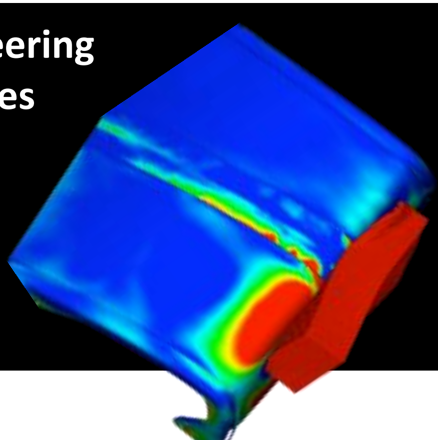
Materials Science

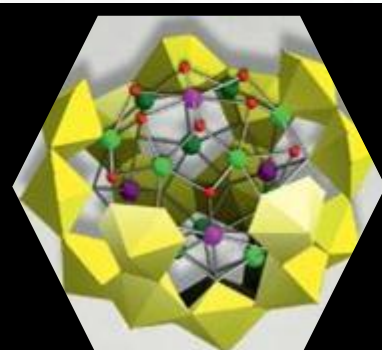


Nanodevices & Microsystems



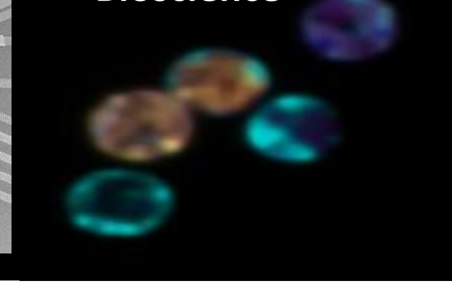
Engineering Sciences





Geoscience

Bioscience



Outline

- Overview
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- Examples of enabling the mission and advancing the frontiers of science and engineering

INTEGRATION OF BLOCK-COPOLYMERS WITH NANO-IMPRINT LITHOGRAPHY

Sandia Principal Investigator: Geoff Brennecka (glbrenn@sandia.gov)

UNM Contact: Professor Steve Brueck (brueck@chtm.unm.edu)

Technical approach

Motivation:

Need 11 nm half-pitch for dense pattern, 4.5 nm critical dimensions (CDs) by 2022

Approach:

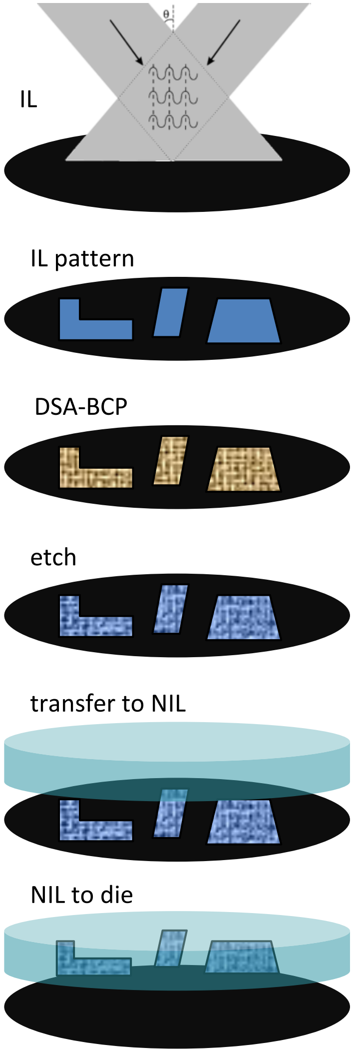
Optical Interference Lithography (IL)

+ Directed self-assembly of block-copolymers (DSA-BCP)

+ Nano-Imprint Lithography (NIL)

Collaboration:

- **Interference Lithography (IL) to define chemical pre-patterns**
  - 70-100nm pitch over large areas
  - Defines where and how BCP self assembly occurs
- **Directed self-assembly of block copolymers (DSA-BCP)**
  - 20-30nm pitch with 10-50 nm CDs today; 4-5nm CDs possible
  - Coupled experiment & simulation
- **NIL to print devices**
  - Stamp with reusable master, no optical constraints
  - <10nm CDs demonstrated



Feasible Large-Scale Nanopatterning

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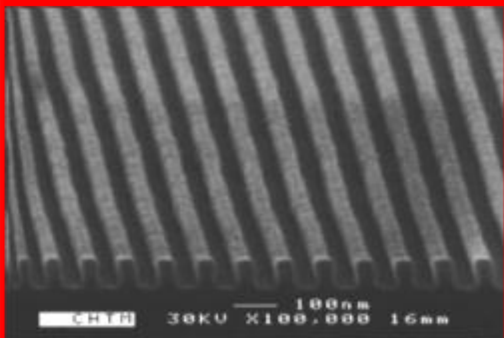
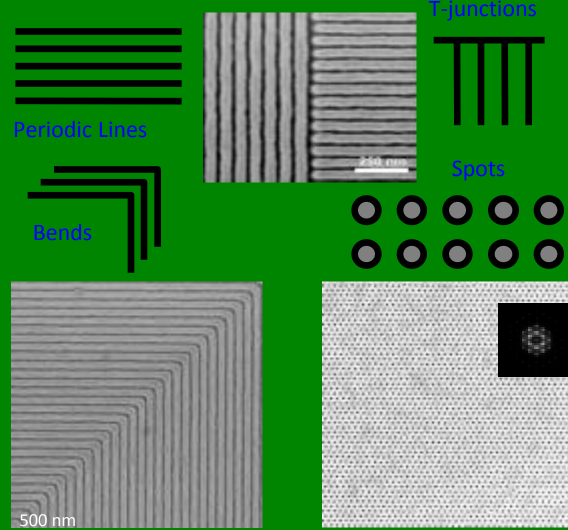
1) <100nm feature definition by IL

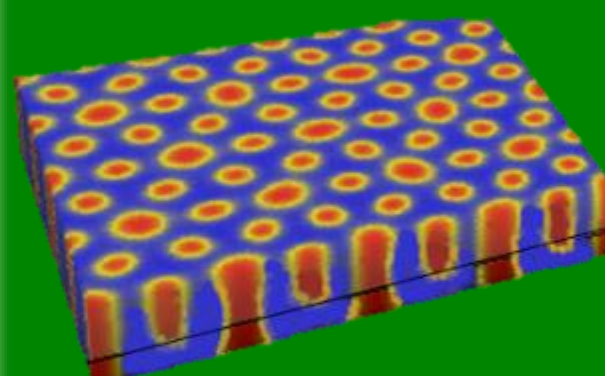


Brueck, Proc. IEEE **93** 1704 (2005)

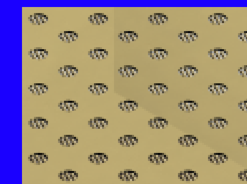
2) BCP self assembly directed by IL to form final 10-50nm features



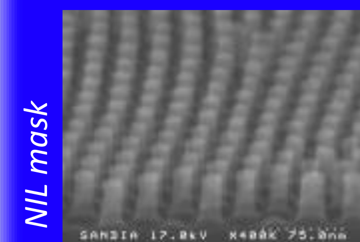
Stoykovich et al. *ACS Nano*, 2007, *Science* 2005

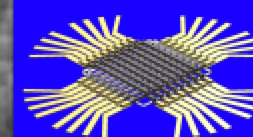


3) Transfer of BCP structures to NIL mask for device-capable patterning



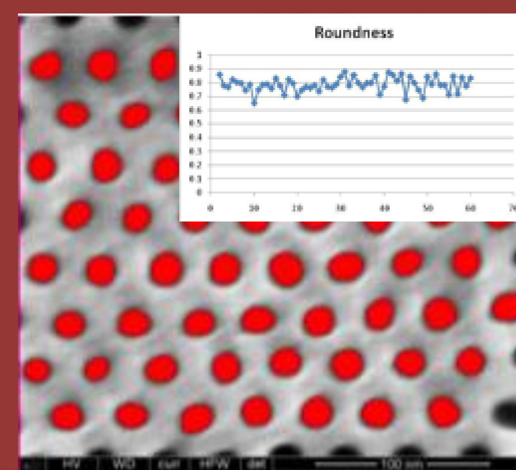
Hybrid 1D/2D plasmonic resonator





Crossbar array

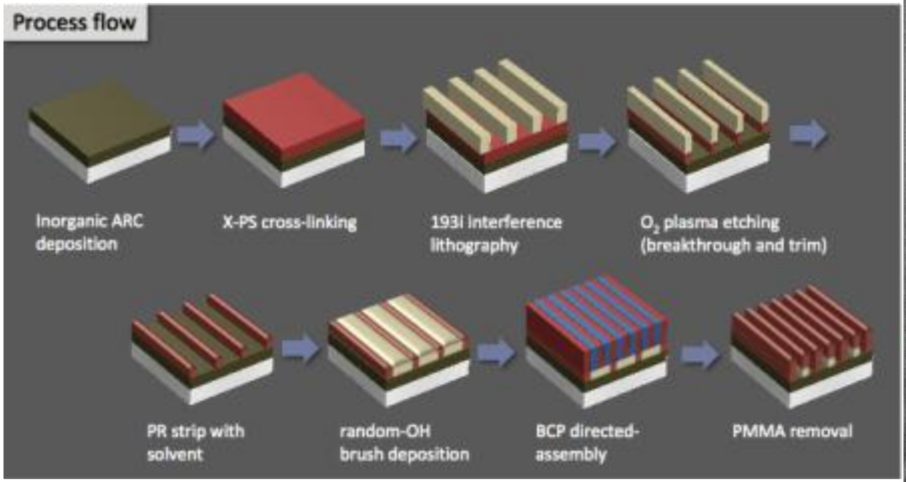
4) Extensive metrology throughout; identify & quantify coupled parameters

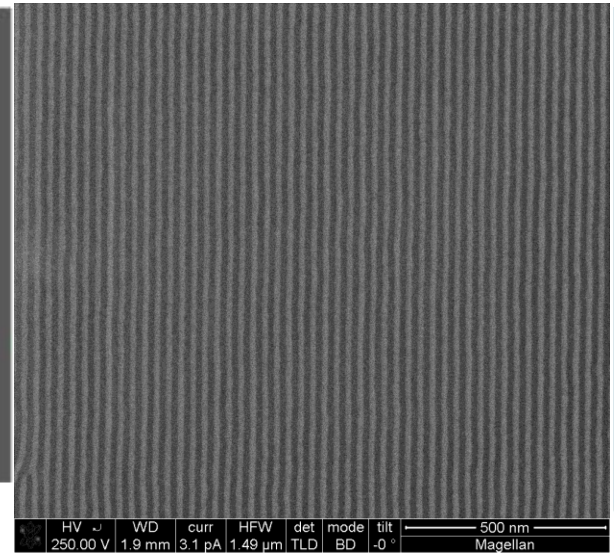


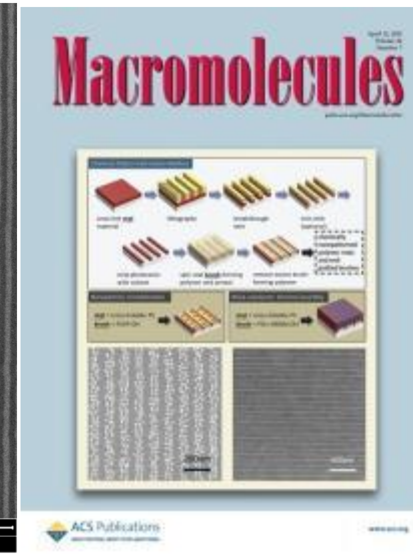
Project Goals:

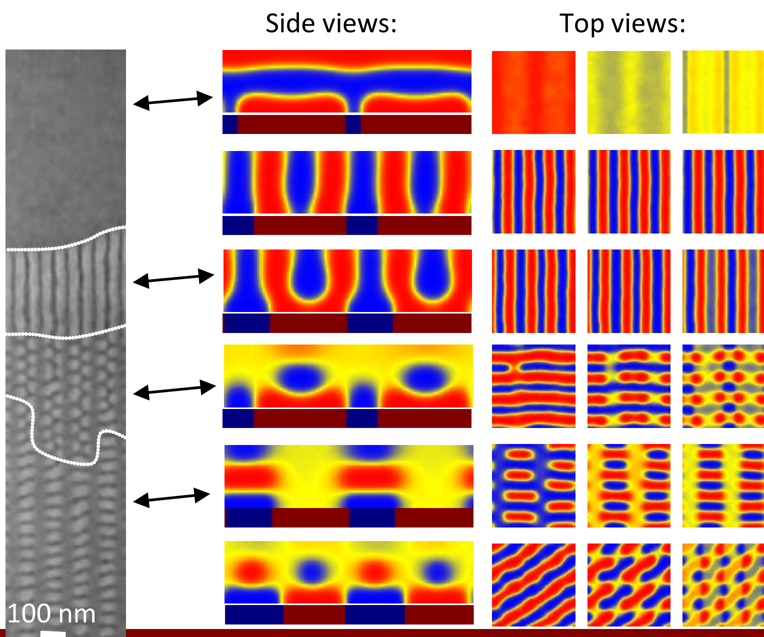
- Science of Directed Self Assembly (DSA)
- Technique integration
- Explore feasibility and limitations of block copolymers (BCP)
- Tool development
- Knowledge & understanding about the techniques and their interactions

Interference Lithography (IL) Directed Self Assembly of Block Copolymers









Results:

- Development of cross-linkable polymer brush layers compatible with IL anti-reflection coatings
- 4x density multiplication of IL patterns across large areas via DSA-BCP
- Improved understanding of surface and sub-surface morphology
  - => insight into surface and interaction tuning
  - Coupling simulation & experiment is critical

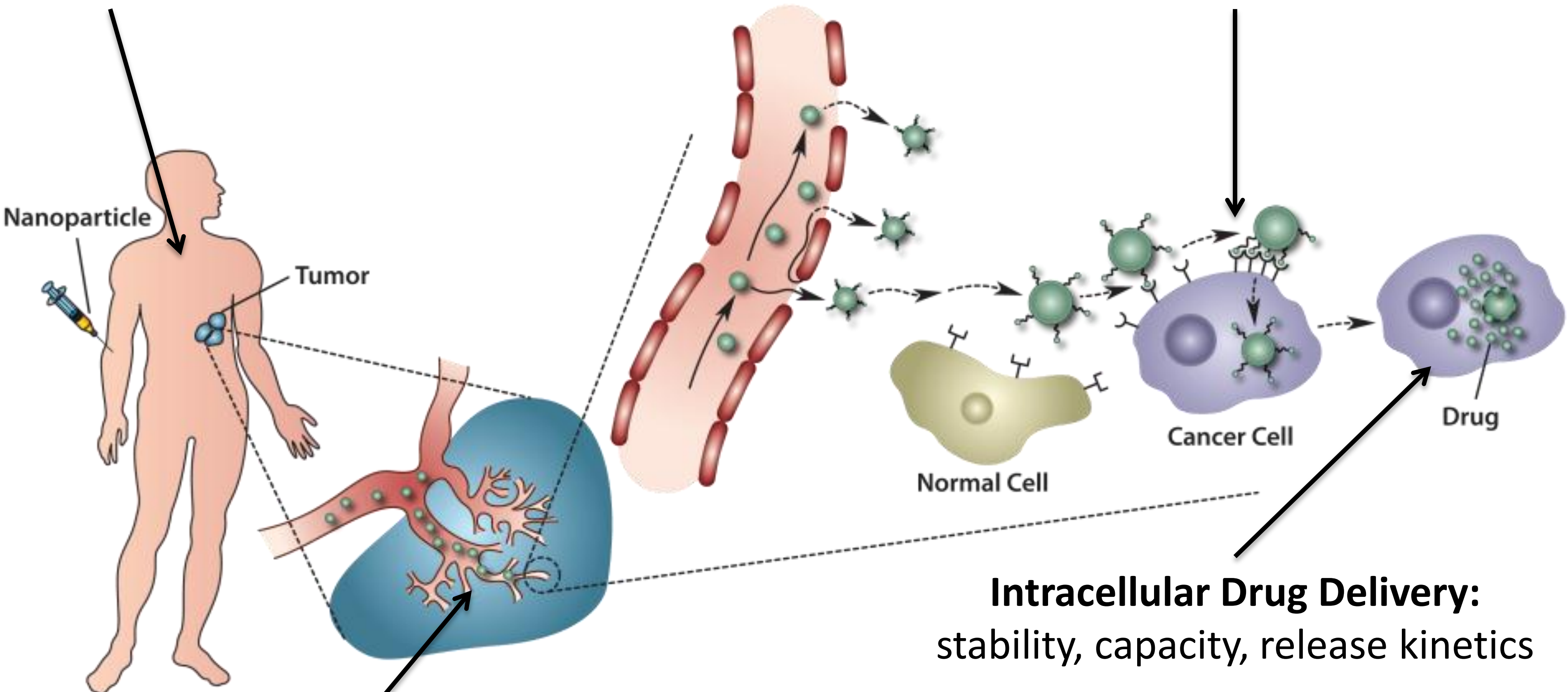
ENGINEERING NANOPARTICLES FOR TARGETED DRUG DELIVERY

Sandia Principal Investigator: Carlee Ashley (ceashle@sandia.gov)
UNM Contact: Professor Jeff Brinker (cjbrink@sandia.gov)

Engineering Nanoparticles for Targeted Drug Delivery

Time in Circulation: shape, charge, surface modification(s), size

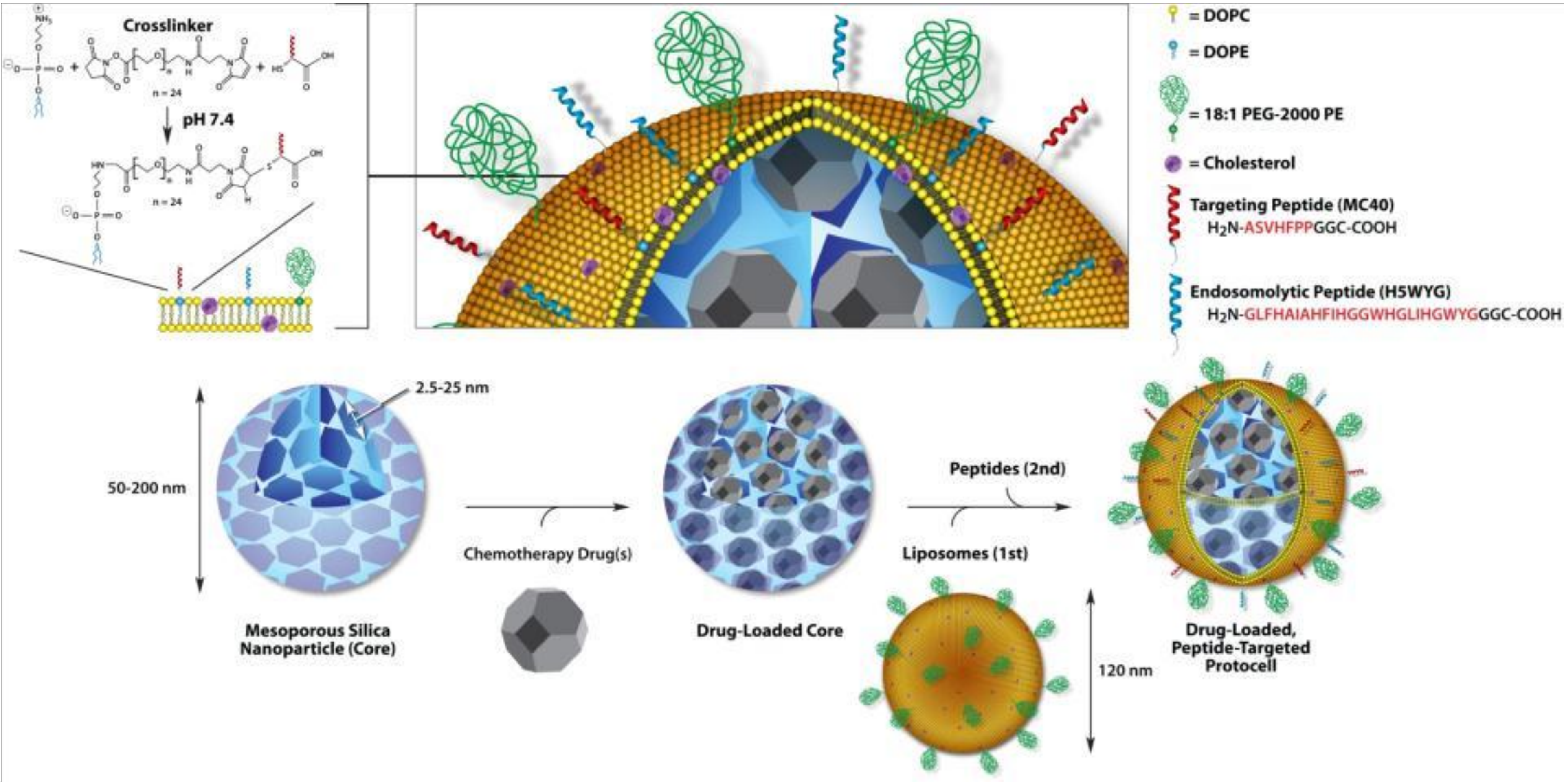
Selective Binding & Internalization: type & density of targeting ligand(s), size, charge, shape



Intracellular Drug Delivery: stability, capacity, release kinetics

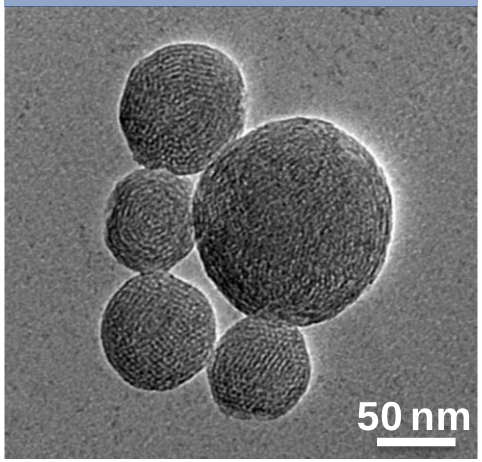
Penetration into Tumor(s): shape, charge, surface modification(s), size

Synthesis of Mesoporous Silica Nanoparticle-Supported Lipid Bilayers ('Protocells')



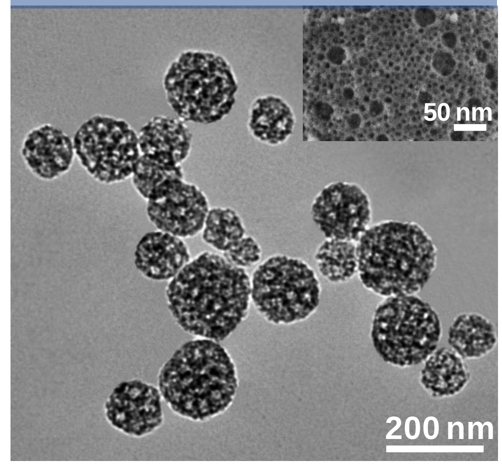
Pore Size/Chemistry and the Degree of Silica Condensation Control Loading and Release of Drugs

Small Pores

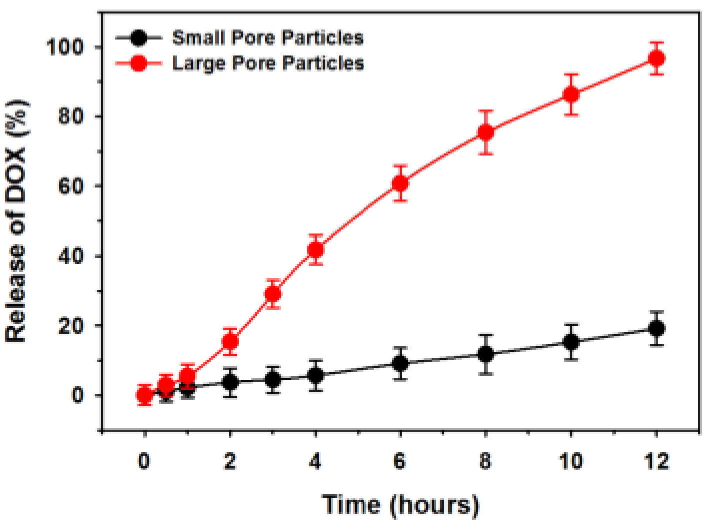


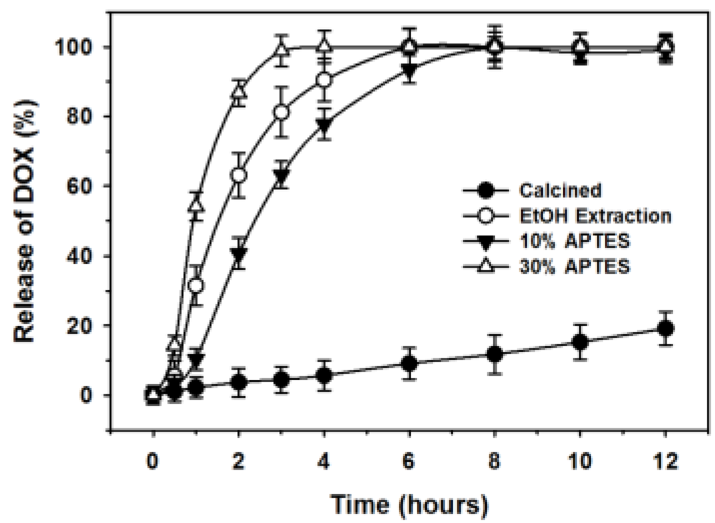
- High surface area (> 1200 m^2/g)
- 2.5-nm pores
- Ideal for delivery of drugs and drug cocktails

Large Pores



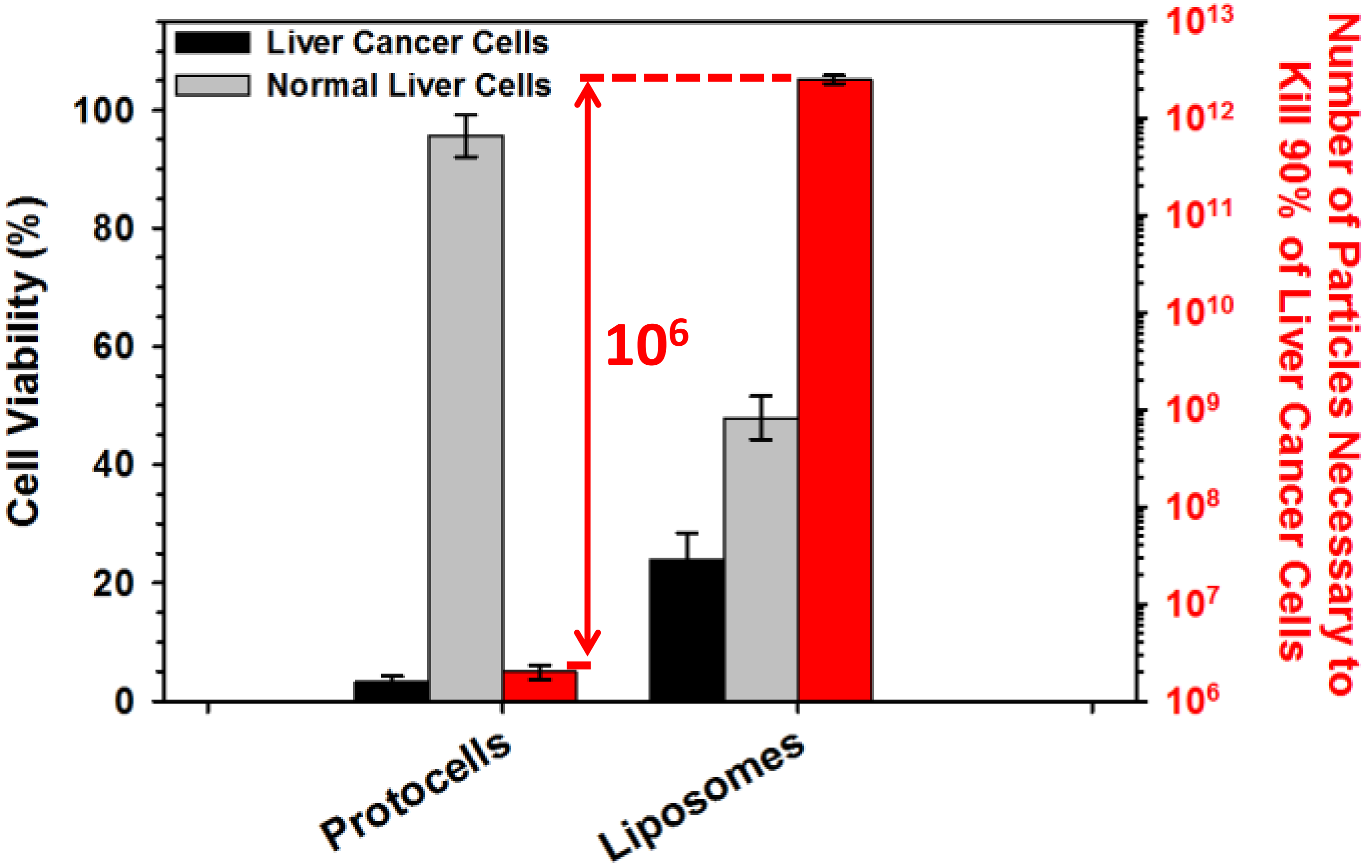
- 15-25 nm, surface-accessible pores
- Well-suited for delivery of nanoparticles, siRNA, plasmids, & mixtures thereof





Release rates depend on pore size and degree of condensation

Targeted Protocells Effectively Kill Liver Cancer Cells Without Harming Normal Liver Cells



Protocells combine a high capacity for drugs, high targeted specificity at low peptide densities, and long-term bilayer stability that is independent of SLB composition.
ONE protocell is sufficient to kill a drug-resistant liver cancer cell

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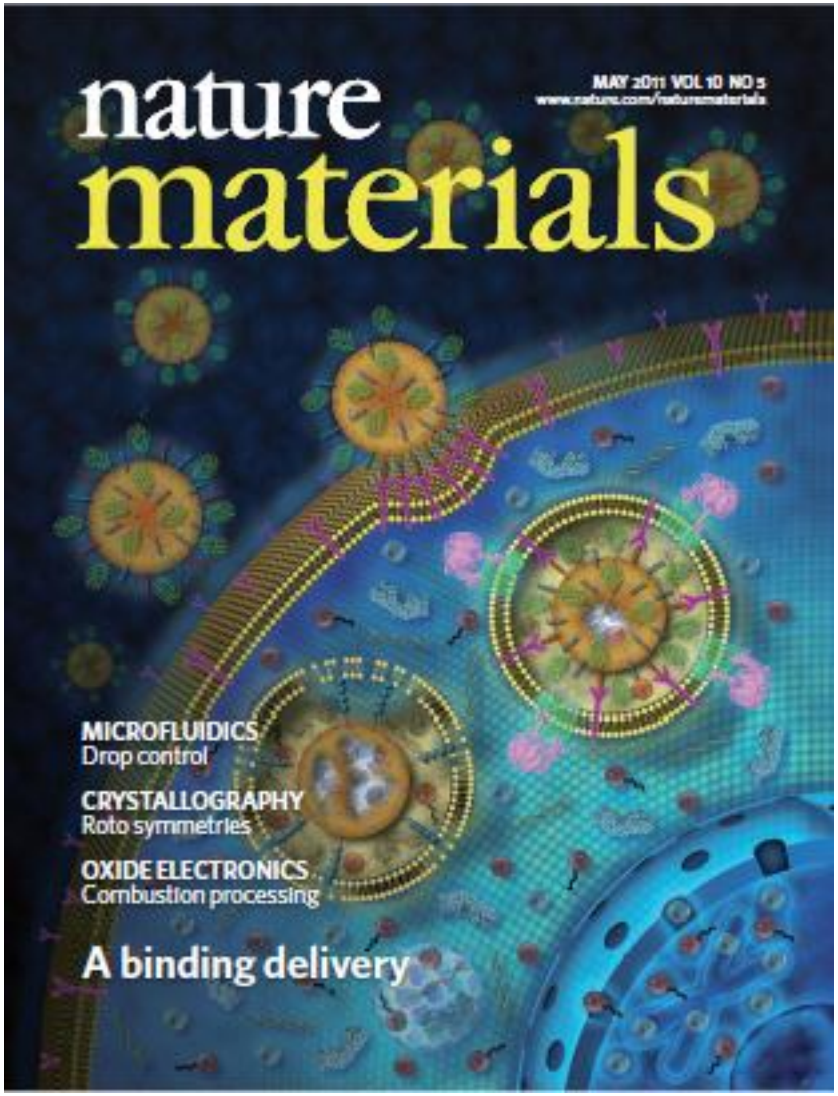
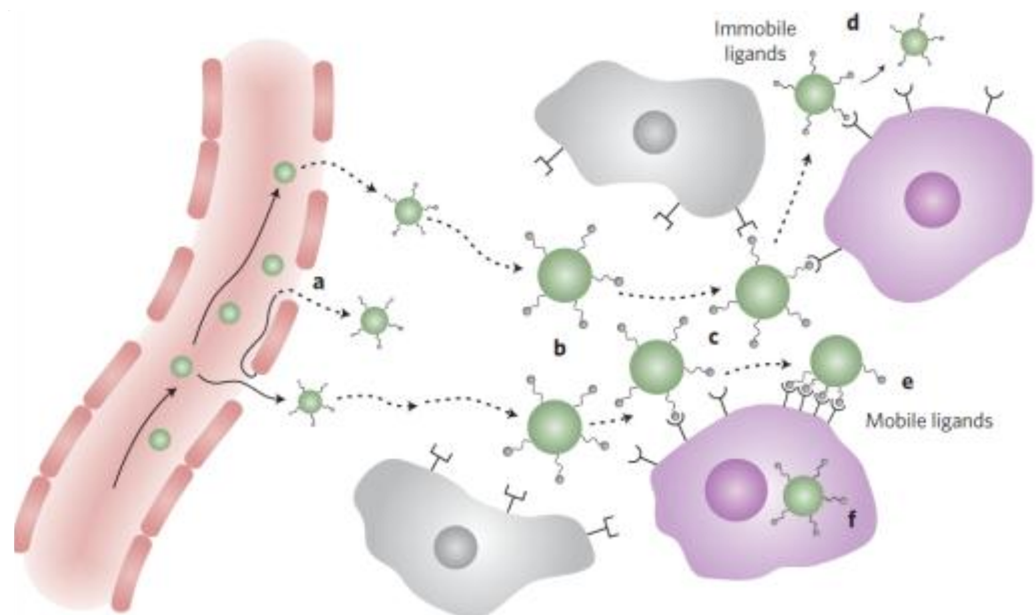


NATURE MATERIALS | NEWS AND VIEWS

Drug delivery: One nanoparticle, one kill

Darrell J. Irvine

Nature Materials **10**, 342–343 (2011) | doi:10.1038/nmat3014
Published online 17 April 2011



The targeted delivery of multicomponent cargos to cancer cells by nanoporous particle-supported lipid bilayers. C. Ashley, J. Brinker, *et al*. *Nature Materials* **10**, 389-397 (2011)

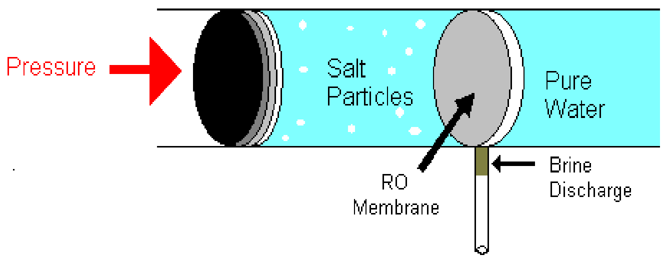
COMPUTATIONAL MATERIAL SCIENCE FOR DESAL MEMBRANE DESIGN

Sandia Principal Investigator: Susan Rempe (slrempe@sandia.gov)
UNM Contact: Professor Jeff Brinker (cjbrink@sandia.gov)

Desalination: A Global Crisis

Half the world lacks clean water

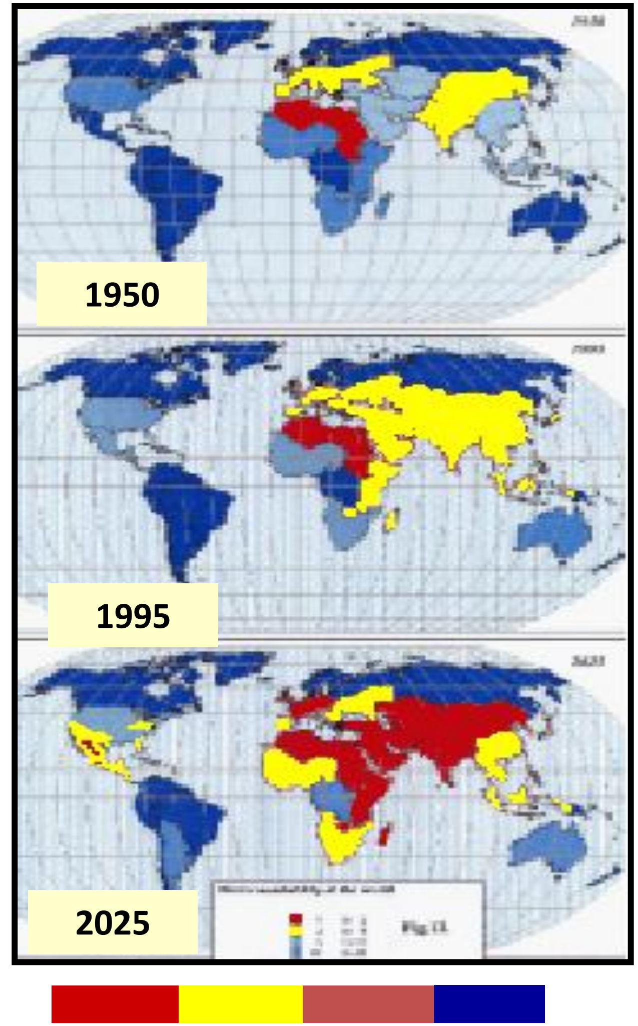
- reverse osmosis technology is expensive
- produces unhealthy water (99% electrolyte-free)



Breakthrough needed in membrane design

- Current design since 1970’s
- need faster water + selective ion exclusion

> **“Water promises to be to the 21st century what oil was to the 20th century: the precious commodity that determines the wealth of nations.”**
>
> *Fortune Magazine, May 15, 2000*

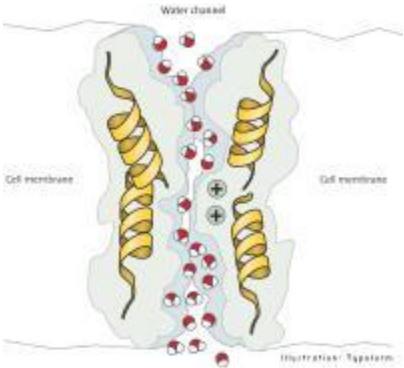


shortage

Efficient Membranes: Mimic Channel Proteins

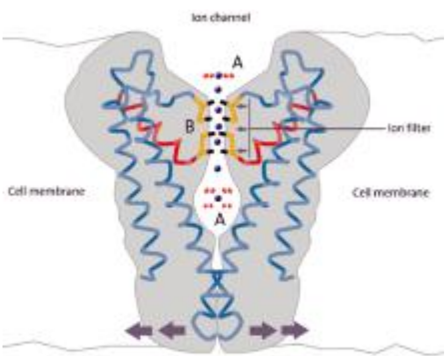
Understand, design, engineer nano-channels for desalination

Water channels



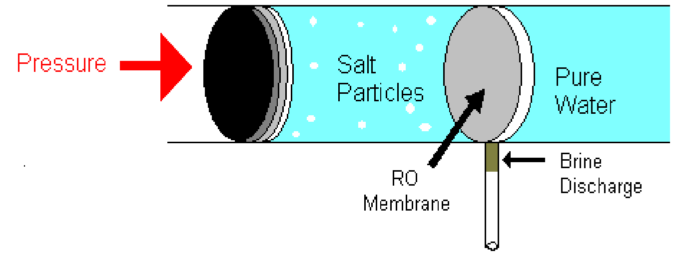
- transport H_2O fast

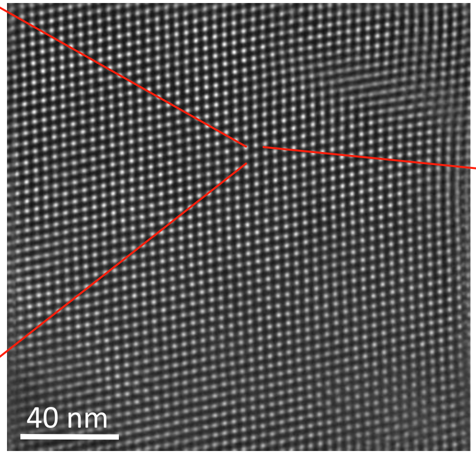
Ion channels



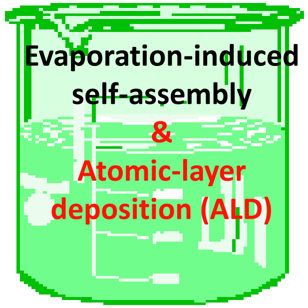
- select minerals fast

- Bio-inspired design
- Theory to reveal mechanism





- Membrane synthesis & function evaluation



Solution: Harness molecular biomechanisms.
Gain 100x in water flux + minerals.

Modeling Identifies Key Structural Features:

Fast water transport & ion rejection

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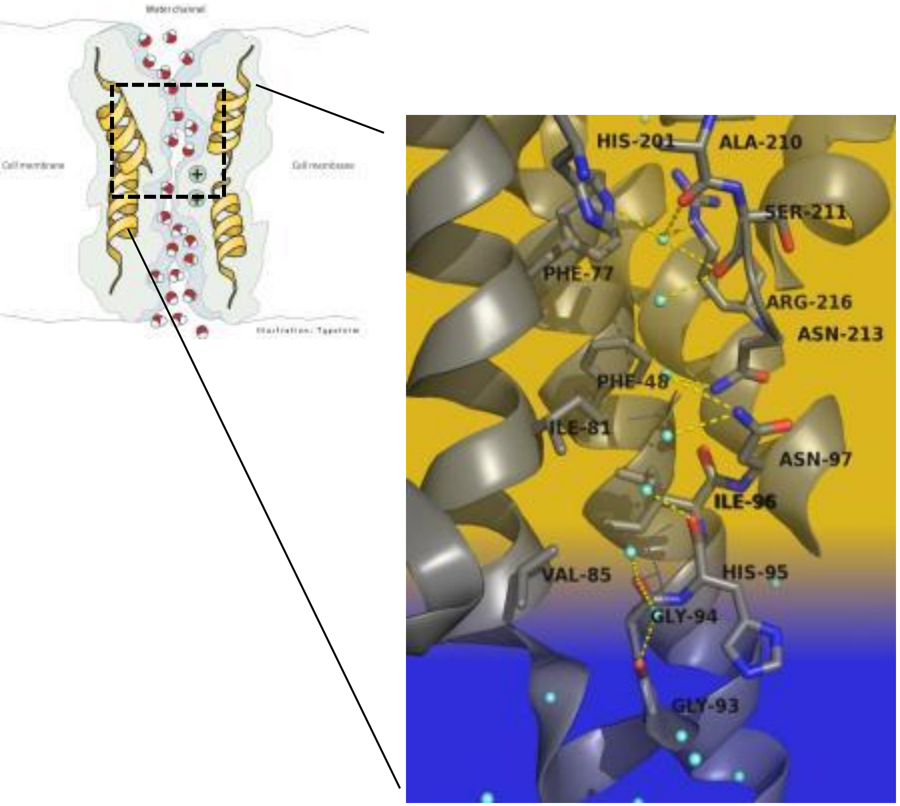
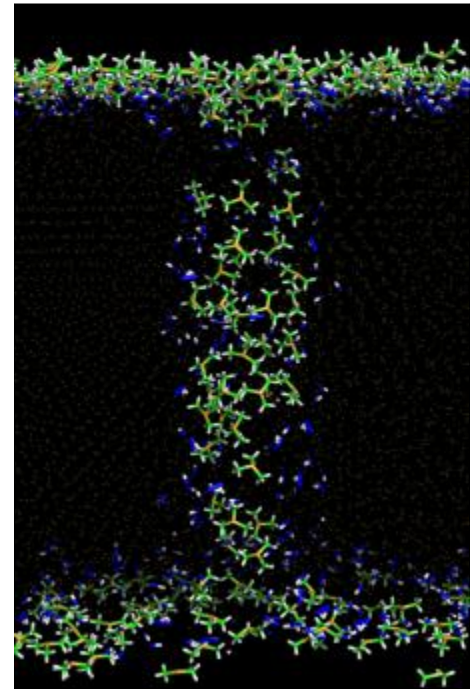


Bio water channel (crystal structure)

(www.nobelprize.org)



Model inorganic pore (simulation results)

(*Phys Rev. Lett* 2006, *J Comp Theor Nanosci* 2009, 2010)

- narrow passageway
- repulsive hydrophobic walls (rings)
- staircase of stabilizing dipoles (C=O, N-H)
- no symmetric dipole clusters

- **over 1 nm** stabilizes ions
- **hydrophobic** walls destabilize ions, but immobilize waters
- **symmetric dense dipoles** bind cations **or** anions

Atomic-layer deposition of polypeptides:

Translates key designs & realizes higher desal efficiency

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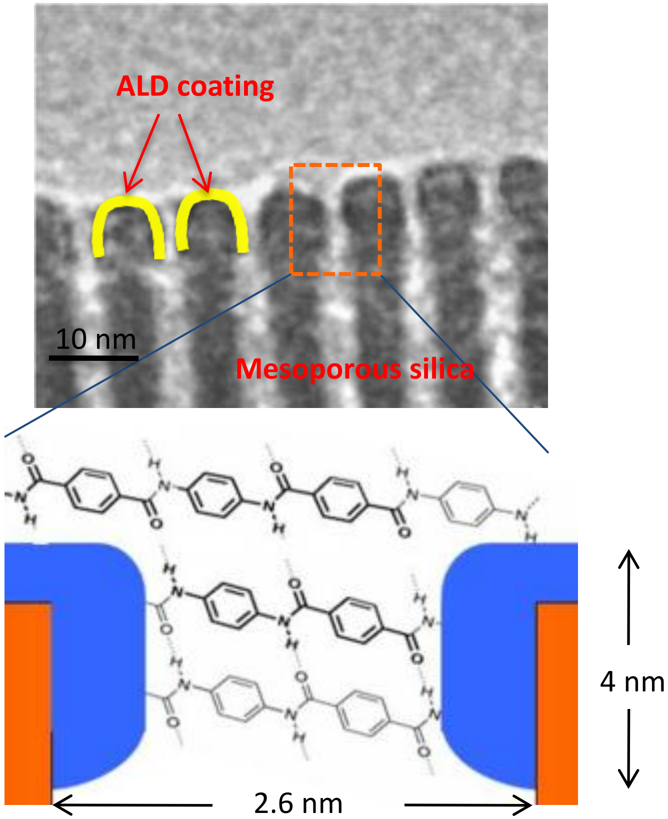
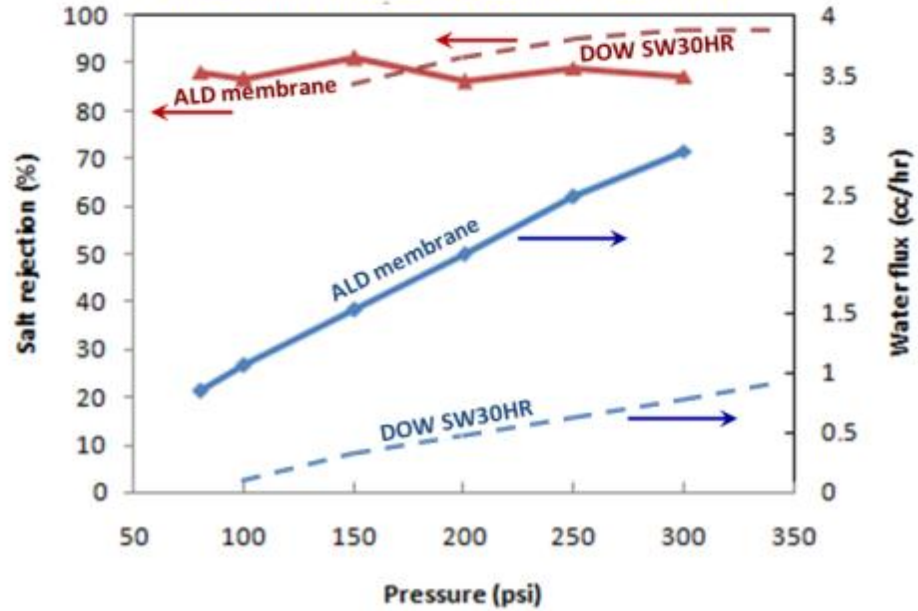


- **C=O**, **N-H** dipoles stabilize water
- **hydrophobic** rings prevent sticking
- **no** symmetric dipole clusters for ions
- **narrow** passageway excludes hydrated ions

Biomimetic (ALD) *vs.* DOW

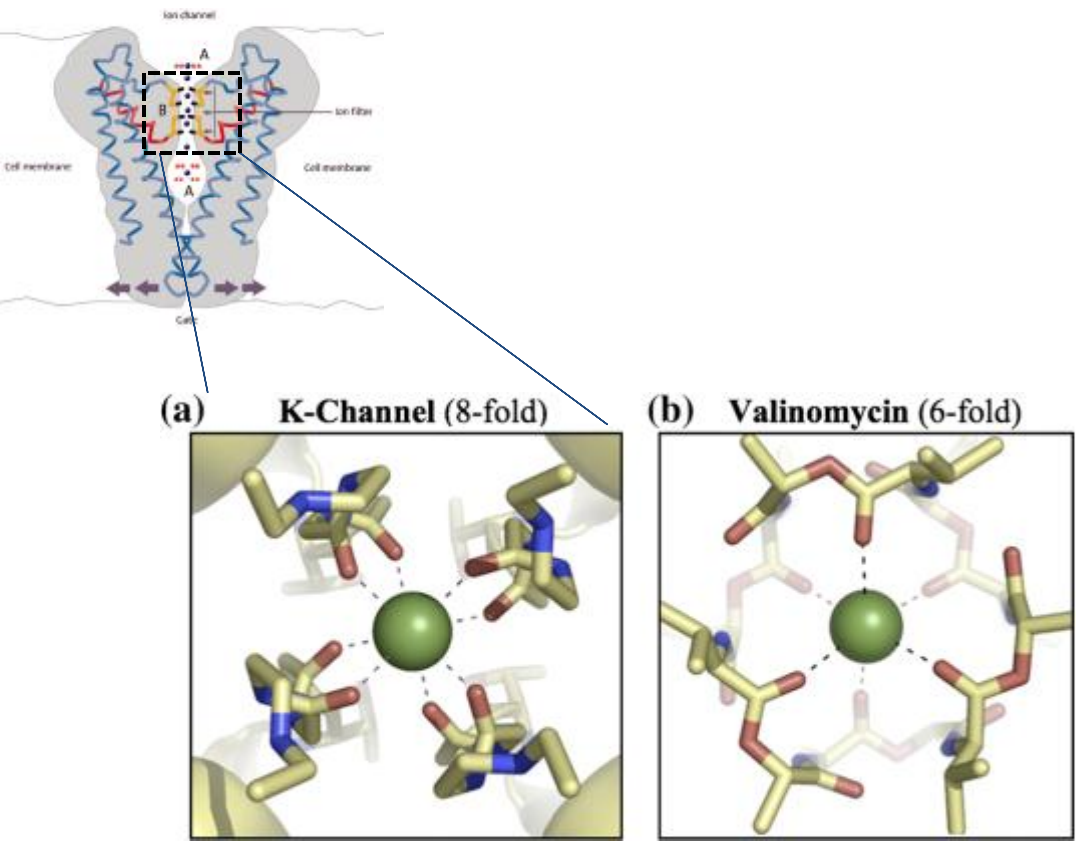


- **10x higher flux** at low applied pressure
- biomimetic design more **efficient**

Provisional Patent #SD-1175
Award for Excellence, LDRD (2010)
Corning Interest
R&D 100 Award, 2011 (R&D Magazine)

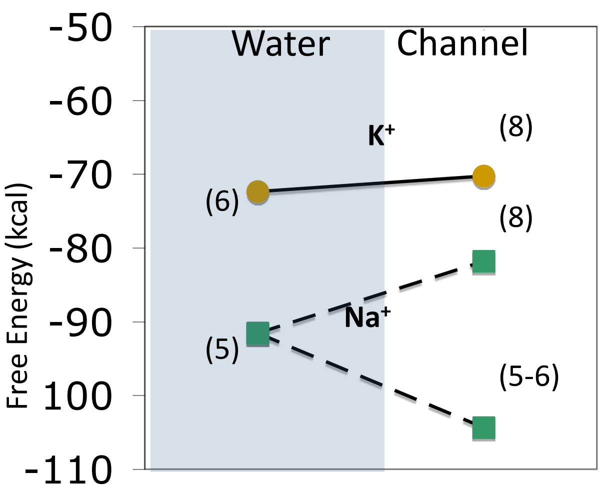
Modeling Identifies Key Structural Features:

Fast transport of select ions + water



1) Over-coordinated binding sites tuned by **surrounds**

2) Specific cavity size in **binding site**



• K^+ selective

• Not selective

Biophys J (2007 & 2010)
J Mol Bio (2008)
J Am Chem Soc (2008)
J General Physiology (2011)

Subtle structure-function relationships resolved by simulation & verified by experiments. Can we translate to inorganic pores?

Computational Materials Science for Selective Membrane Design

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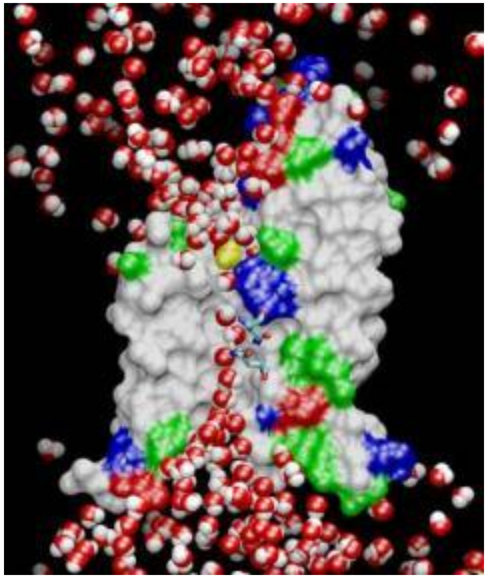
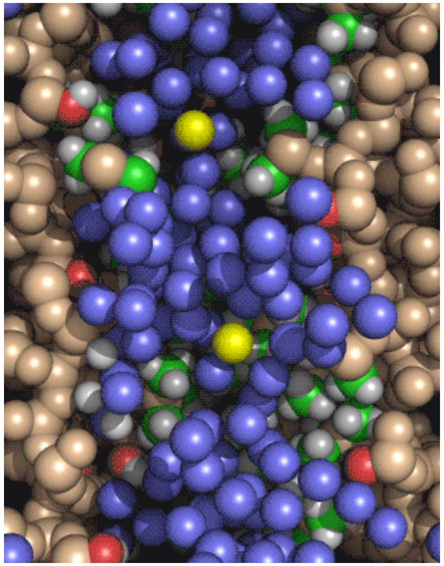
Biological Water Channel



(Tajkhorshid & co)

Bio mechanisms → Engineering solutions

Inorganic Water Channel



(Desal Team, Sandia)

Solve important material design problems by understanding & mimicking nature:

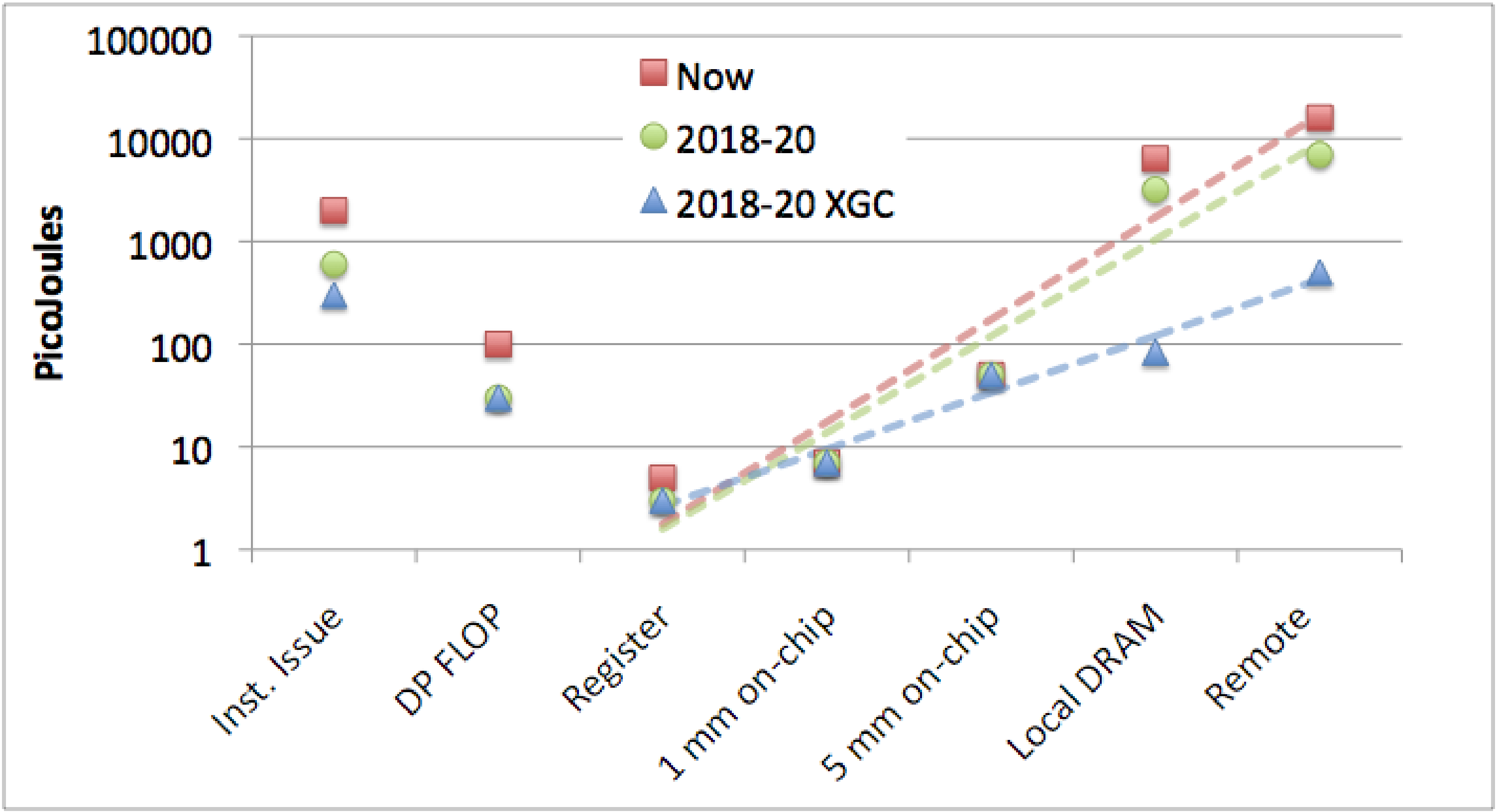
- **Water-Energy** (mineral water, efficiently)
- **Energy-BioBatteries** (charge separation, fast, selective transport)

Biology ⟷ inorganic nanostructures
Quantum modeling ⟷ experiments

EXASCALE GRAND CHALLENGE

Sandia Principal Investigator: Rich Murphy (rcmurph@sandia.gov)

Exascale Grand Challenge Problem and Vision

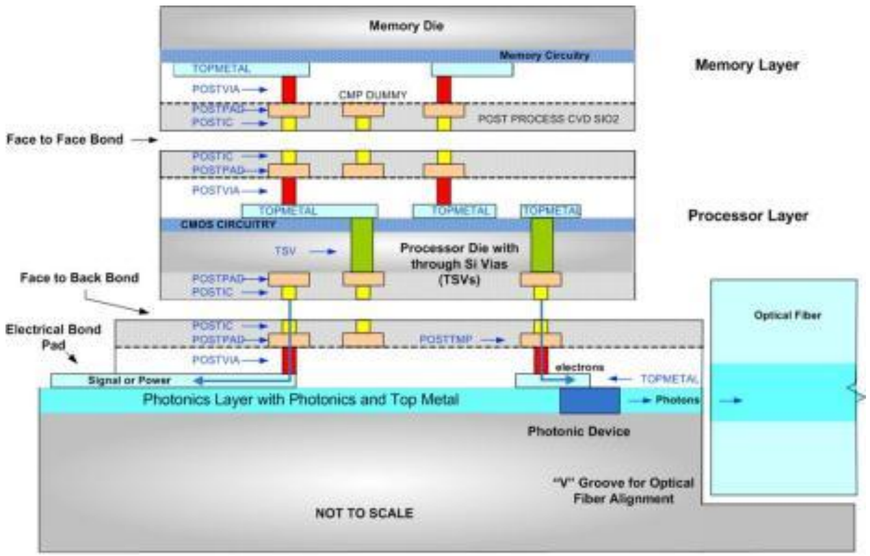


Take the first steps to enable low-energy computing at tera-, peta-, and exascale to benefit DOE and DoD mission applications

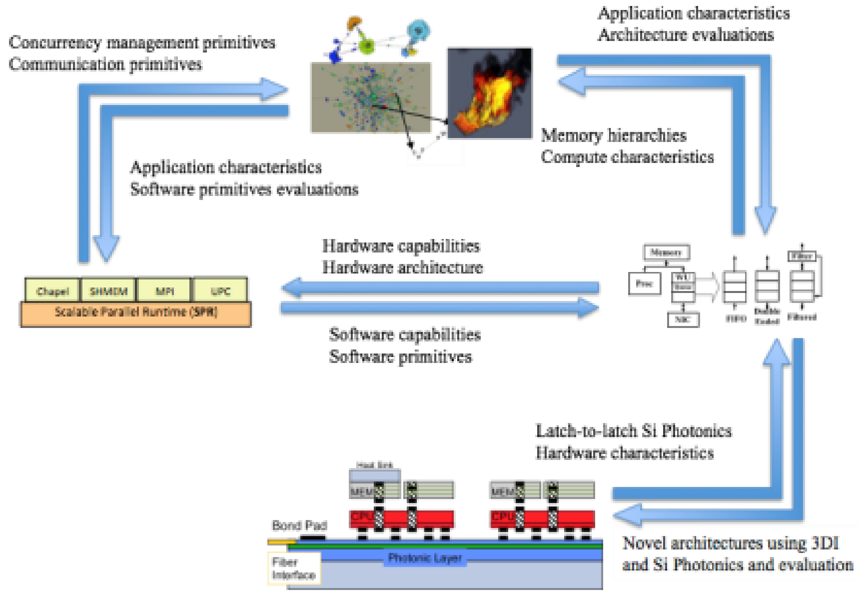
- Focus on Data Movement, not computation
- Vertically Integrated Tradeoffs in 4 Thrusts: Applications, Systems Software, Architecture, and Microelectronics

Exascale GC "Holy Grail"

Enabling Technologies



Impact Through Codesign



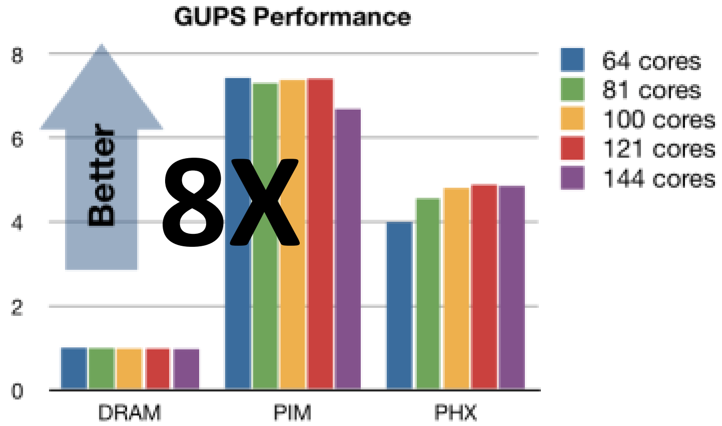
- Enabling Technologies:
  - 3D Integrated Logic, Memory, and Silicon Photonics on a single package
  - Significantly reduced communication energies at short and long distances
- Impact on Mission Applications
  - Redesign the system to match the enabling technologies and application requirements
  - Modern processors are designed around poor (high latency, low bandwidth) communication technologies

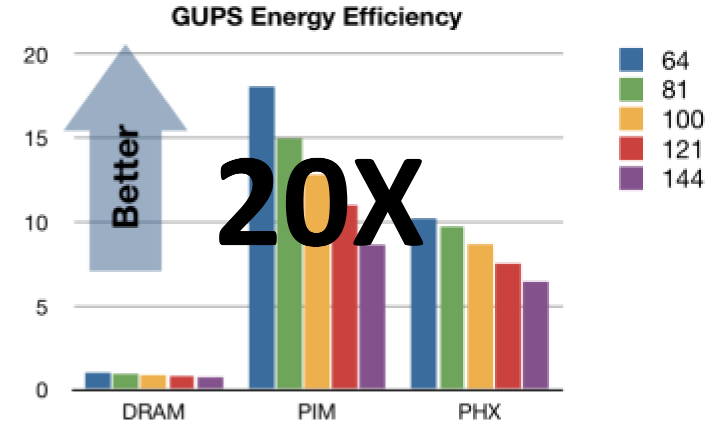
Early Results

Sandia National Laboratories

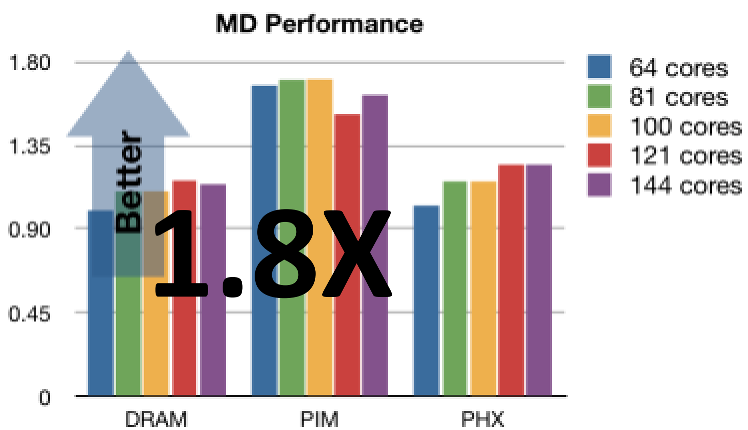
Performance | Energy Efficiency

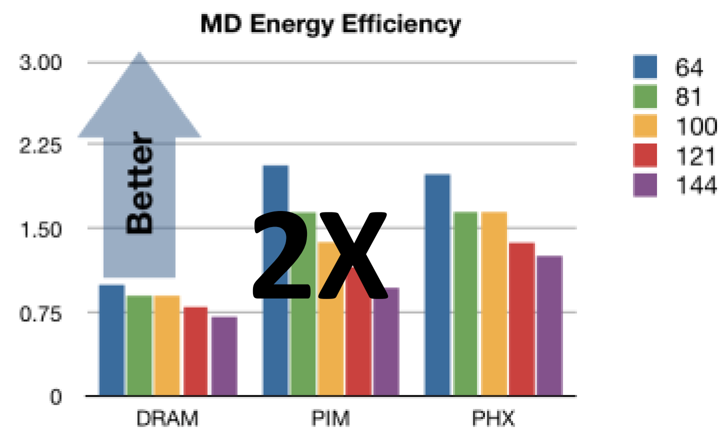
GUPS





MD



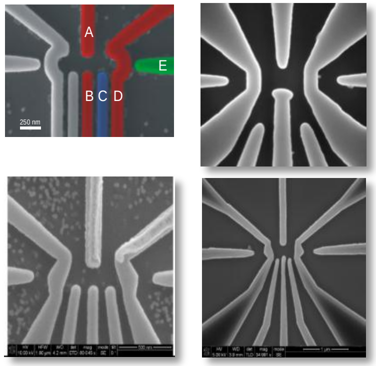


AQUARIUS GRAND CHALLENGE

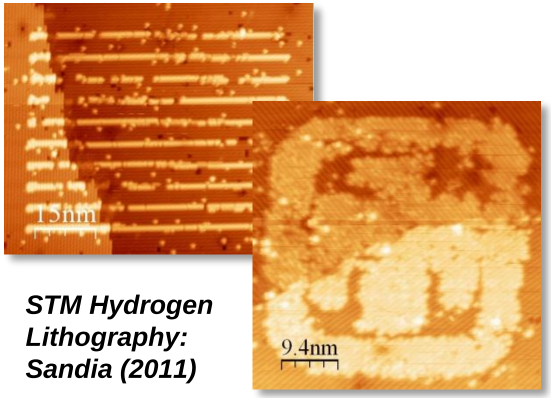
Sandia Principal Investigator: Andrew Landahl (ajland@sandia.gov)
UNM Contact: Professor Ivan Deutsch (ideutsch@unm.edu)

AQUARIUS Grand Challenge

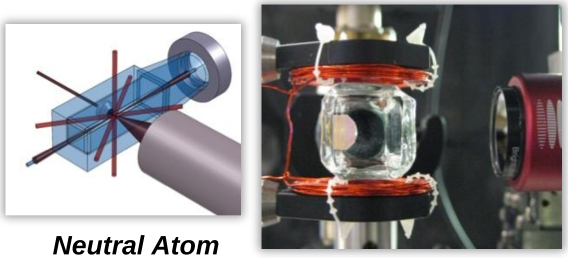
- Goals
  - Demonstrate special-purpose two-qubit adiabatic quantum computing (AQC) optimization algorithms in neutral atoms trapped by a nanofabricated optical array and electrons trapped by silicon nanostructures
  - Assess potential for universal fault-tolerant AQC architectures
- Accomplishments
  - Demonstration of isolated silicon “charge” qubit
  - Demonstration of atomic-scale Silicon lithography
  - World-first fabrication of diffractive optical elements for Cesium atom trapping and control
  - World-first trapping of three separated Cesium atoms
  - Operation of Sandia’s first quantum processing device



Quantum Dots: Sandia (2011)



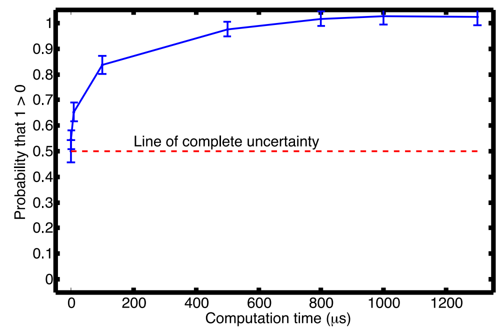
STM Hydrogen Lithography: Sandia (2011)

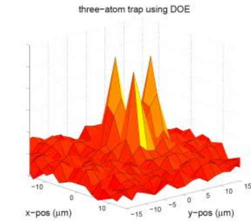


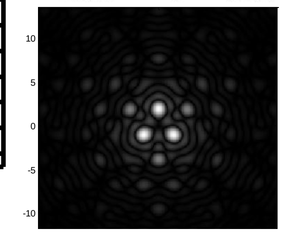
Neutral Atom Experiments

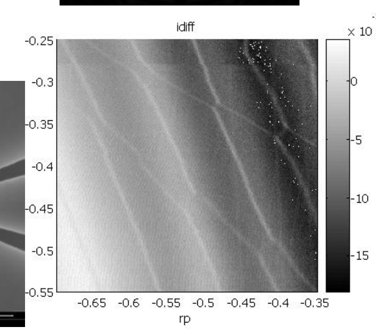
Additional Technical Accomplishments

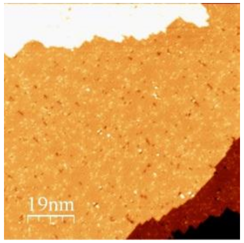
- Neutral Atoms:
  - Sandia's first quantum calculation: 1 is greater than 0!
  - Updated atomic physics calculations per External Advisory Board suggestions; joint SNL-UNM paper forthcoming
- Semiconductors:
  - First PH_3 incorporation in an atomic-precision fabrication system completed; initial testing underway
  - Double Quantum Dot (DQD) advances:
    - Single DQD charge qubit in demonstration and testing
    - DQD-DQD structures fabbed and in test; indications of Coulomb blockade and tunability
  - Deployed architecture team's adiabaticity "smoking gun" experimental protocol: in progress
- Architecture:
  - Constructed adiabatic quantum computing-compatible error detection codes
  - Performed feasibility study for ground state quantum computing
  - Developed "smoking gun" experimental protocol to distinguish adiabaticity from relaxation

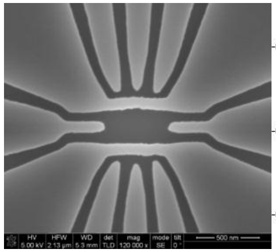


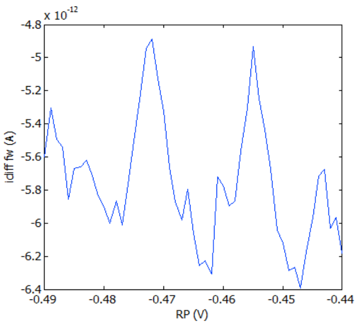


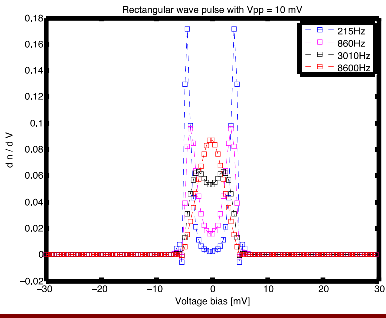












RETROSPECTIVE

Impact – Micro ChemLab Grand Challenge
(one of the first GCs)

Challenge: Develop systems for the detection of chemical agents and biological threats in environmental and clinical settings that are rapid, portable, automated, and highly accurate

LDRD Origin: **13 projects over 15 years, of which 3 were GCs**

- Autonomous Microchem Laboratory - µChemLab™ Grand Challenge
- Microscale Immune Studies Laboratory Grand Challenge
- Molecular Integrated Microsystems (MIMS) Grand Challenge
- Rapid Threat Organism Recognition (RapTOR) Grand Challenge

Additional R&D Investments:

- NIH
- NASA
- DHS
- DoD
- DARPA
- DTRA
- CBNP (DOE)
- NA-22 (DOE)
- Intelligence Community

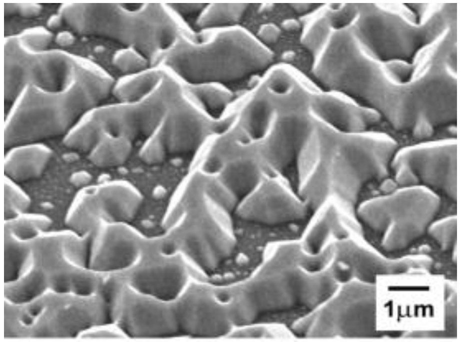
Mission Impact:

- Portable, point-of-care diagnostics systems for public health, warfighter protection
- Biodosimetry platform co-developed with Armed Forces Radiological Research Institute
- Research platforms for use in constrained environments (such as high-biothreat field labs)
- Military intelligence, force protection, U.S. chemical stockpile disposal
- Nonproliferation, civilian toxic industrial chemical incident response, environmental monitoring
- Automated molecular biology (AMB) platform

Impact – Solid State Lighting Grand Challenge

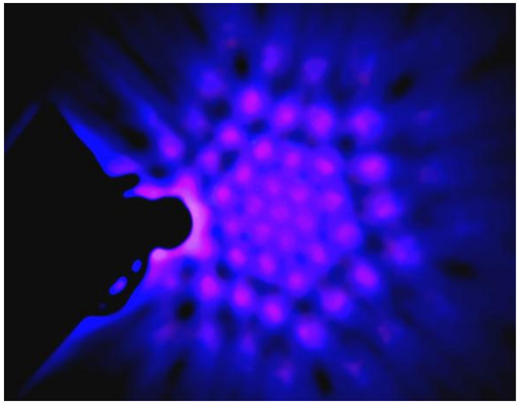
Challenge: Improvements in energy efficiency of lighting, which consumes 22% of US electricity and 6.5% of US primary energy. Also UV LEDs for bio-sensing and non-LOS communications.

LDRD Origin:
- S&T Base for Ultra-Efficient Solid State Lighting & Synergistic National Security Needs Grand Challenge
- UV Lasers

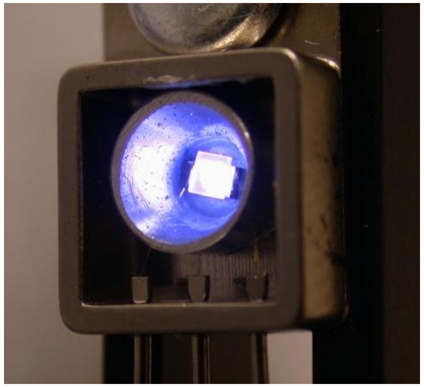


Controlled GaN nucleation layers

Additional R&D Investments:
- 14 DOE/EERE projects on SSL, many joint with industrial partners
- 3 DARPA projects (UV light emitters)
- 1 DOE BES Core Program project
- Energy Frontier Research Center for SSL ($18M over 5 years)
- Projects for NW and NS customers


Photonic Crystal LED

Mission Impact:
- Accelerated development and adoption of SSL worldwide; helped start DOE's Next Generation Lighting Initiative
- Developed GaN-based optoelectronics for national security applications

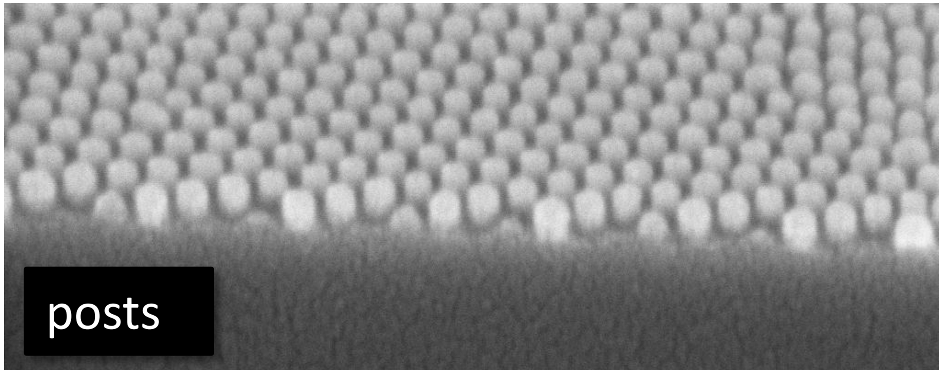

Packaged Deep UV (275 nm) LED

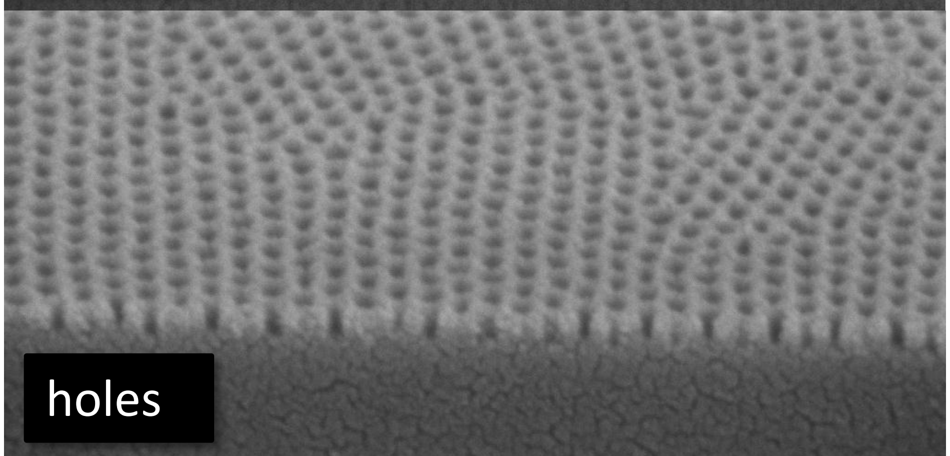
UNM collaborations are valued

- Large cross-section of research is being conducted

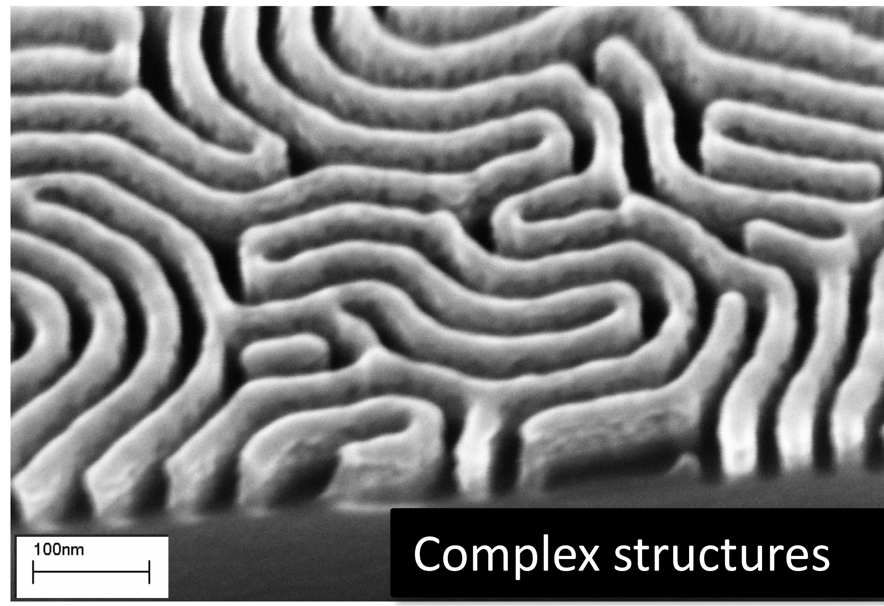
BACKUP SLIDES

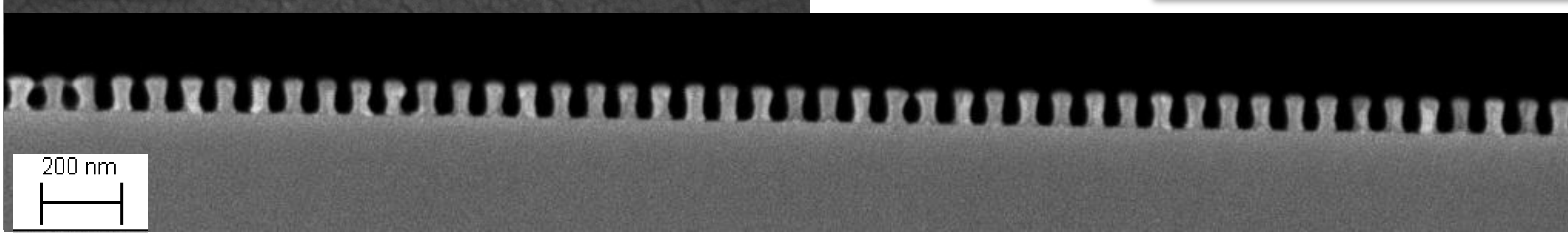
Nanoscale Pattern Transfer





Pattern inversion and mask hardening by ALD infiltration

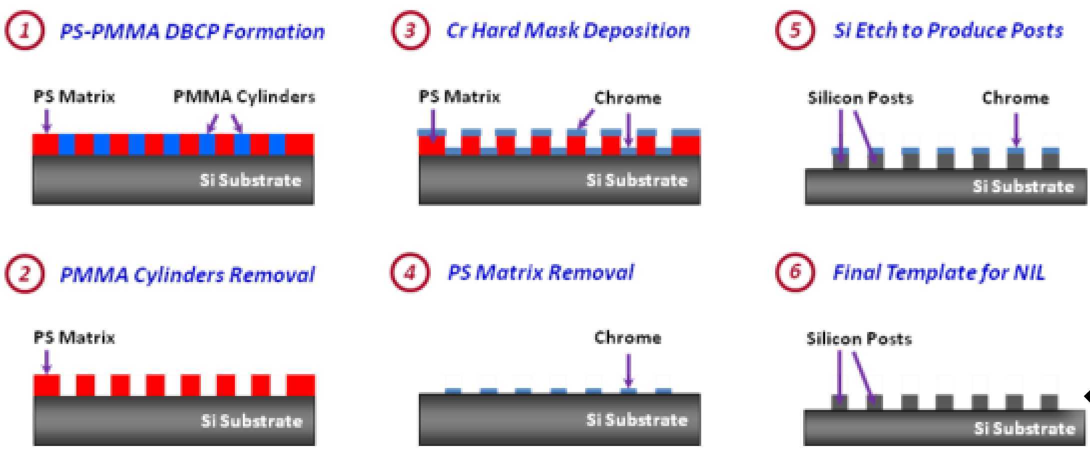


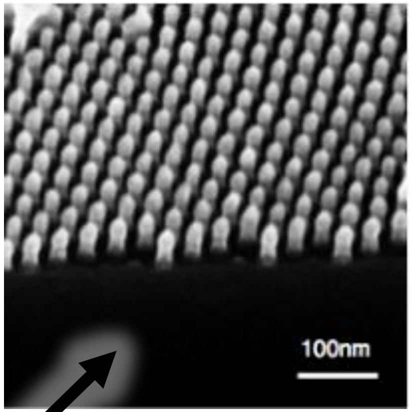


NanoImprint Lithography for Optical and Electronic Device Structures

Sandia National Laboratories

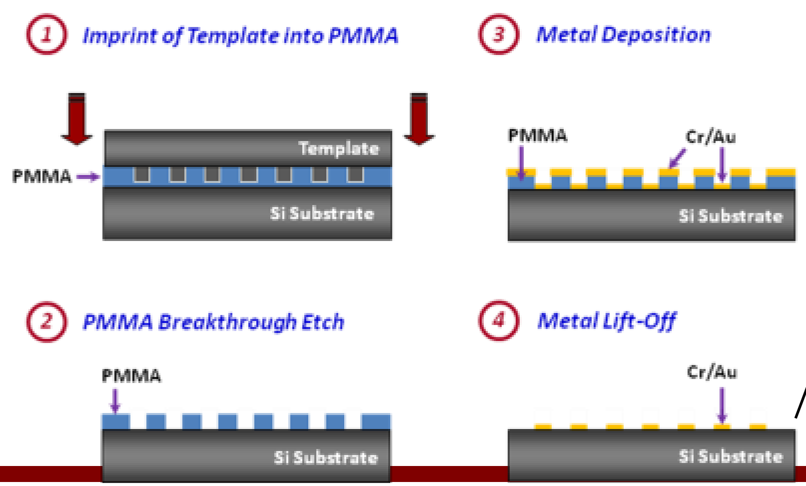
NIL mold via BCP

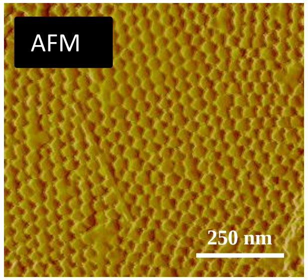


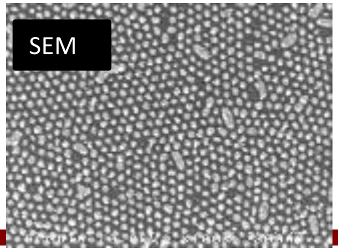


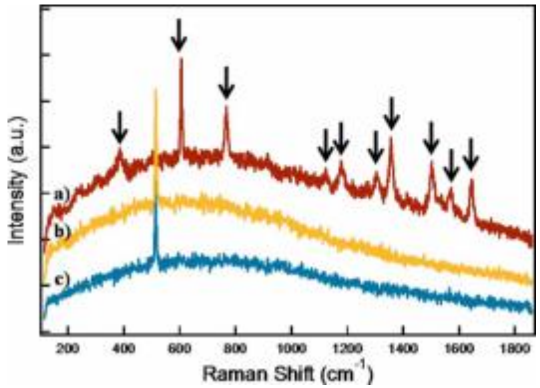
Integration of block copolymer self assembly and nanoimprint lithography presents a more rapid and cost-effective approach to nanofabrication compared to e-beam template writing.

Simple SERS demonstration via NIL









Raman scattering plots of R6G on a) device chip - patterned section, b) control chip - bare silicon, and c) device chip – bare silicon section. Black arrows denote R6G scattering peaks.