MIT-Stanford-Berkeley Nanotechnology Forum

Panel on Emerging Tools and Instrumentation

Organizer: Scott Mize, MIT

Panel

William A. Goddard III, Caltech

Gerhard Goldbeck-Wood, Dir. Nanotech., Accelrys

Maximilian Schroeck, Director, Agilent Ventures

Lewis S. Gruber, CEO Arryx

Lloyd Lacomb, VP Semiconductor products, Veeco

Who is William A. Goddard III?

Charles and Mary Ferkel Professor of Chemistry, Materials Science, and Applied Physics
Director, Materials and Process Simulation Center, Beckman Institute
California Institute of Technology, Pasadena, California 91125
[http://www.wag.caltech.edu]

110 PhD's, 550 papers, Member of the National Academy of Science (1984)
12 patents filed in protein structure prediction, drug design, new polymerization catalysts, semiconducting processing modeling, H_2 storage.
Co-founded 7 companies (all started in Pasadena and still thriving)
Molecular Simulations Inc (1984) now named Accelrys and located in San Diego. molecular dynamics and graphics tools for design of drug and materials, ~360 emp.
Schrodinger Inc (1990). Now in NY city and Portland. Quantum mechanics and drug design tools , 65 emp.
Systine Inc (2000): nanoscale etching tools using low energy electrons, 4 emp.
Eidogen Inc (2000): tools for protein drug targets and leads based on structure from bio-informatics, 24 emp.
Allozyne Inc (2004): therapeutics based on non-natural amino acids (1 emp)
Qateomix Inc. (2004): Rapid prototyping and IP for catalysts with integrated theory and experiment (1 emp).

QUESTION #1: Is Nanotechnology Practical?

When I started working on nanotechnology In 1985, it seemed impossible that experimentalists would ever be able to make the designs that we might come up with

With the very impressive progress in synthesizing and testing nanoscale systems at UCLA, Harvard, MIT, Stanford, Rice, Caltech and elsewhere, I now believe that it will be possible to make practical nanoscale devices and fully expect to see demonstrations before I retire from Caltech.

Question #2: What tools are needed?

I will give some examples from research we are currently carrying out on nanotechnology

QUESTION#3: Where should Funding and investment be directed

Major funding should be dedicated to developing tools deemed essential to demonstrations of the emerging technology to enable small scale manufacturing of functional devices (objective is function not cost)

As systems are discovered with unique functionality, some will provide solutions that can justify the higher costs using current technology, providing a means for the increased production that eventually will lower the costs to acheiving practical nanotechnology

Molecular Based Nanotechnology

Central Issues

- **Design** (nanofuelcell, nanoelectronics, analog to digital convert)
- **Synthesis** (need automated self-assembly since cannot see)
- **Characterization, Optimization**
- **Fabrication** (Reproduction)
- **Communication** (getting info to and from nanodevice)
- **Properties** (sensing environment, tribology,)

Paradigms For Synthesis

- **Mech-atomical** [Mechanical Positioning Atoms (AFM, STM)]
- **Self-assembly** (Monolayers)
- **Chemical** (Use Living Catalysts at Specified Sites)
- **Biological** (Use apparatus of living cells to make components but maybe not to assembly the system)

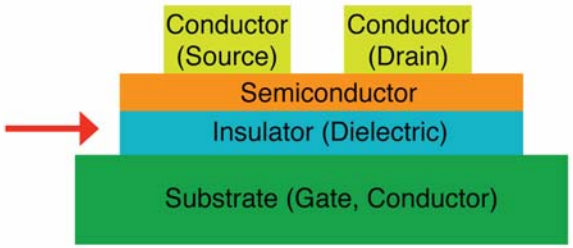
Critical Long-term Problems

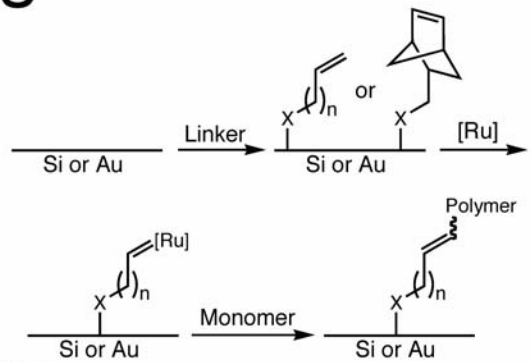
- **Communication** (info to and from nanodevice)
- **Error Detection and Error Correction** (Proofreading)
- **Reproduction** (Self Replication, The Assembler)

Nanodevices using novel Polymer synthesis techniques

Devices

Thin Film Field Effect Transistors (FETs)





- Advantages of SI-ROMP
  - Large area processing, new geometries (conformal layers), material variety, mild conditions, short reaction times, light weight
- Considerations
  - Component layers
    - Spin-coating, lithography, vacuum sublimation
  - Performance requirements
    - Layer compatibility, smooth interfaces, low leakage
  - Benchmark measurements
    - On/off ratio and mobility

Lucent Technologies
Bell Labs Innovations

Oren Scherman and Bob Grubbs, 2004

Essential to Combine Experiment and Theory

- **Opportunity**: Tremendous potential for new functional materials (artificial machines smaller than cells)
- **Problems**:
  - **Synthesis**
  - **Characterization**
  - **Design**
- **In each area there are tremendous experimental challenges.**
- **In each case the time to solution will be dramatically decreased by the use of**

First principles (de novo) simulations

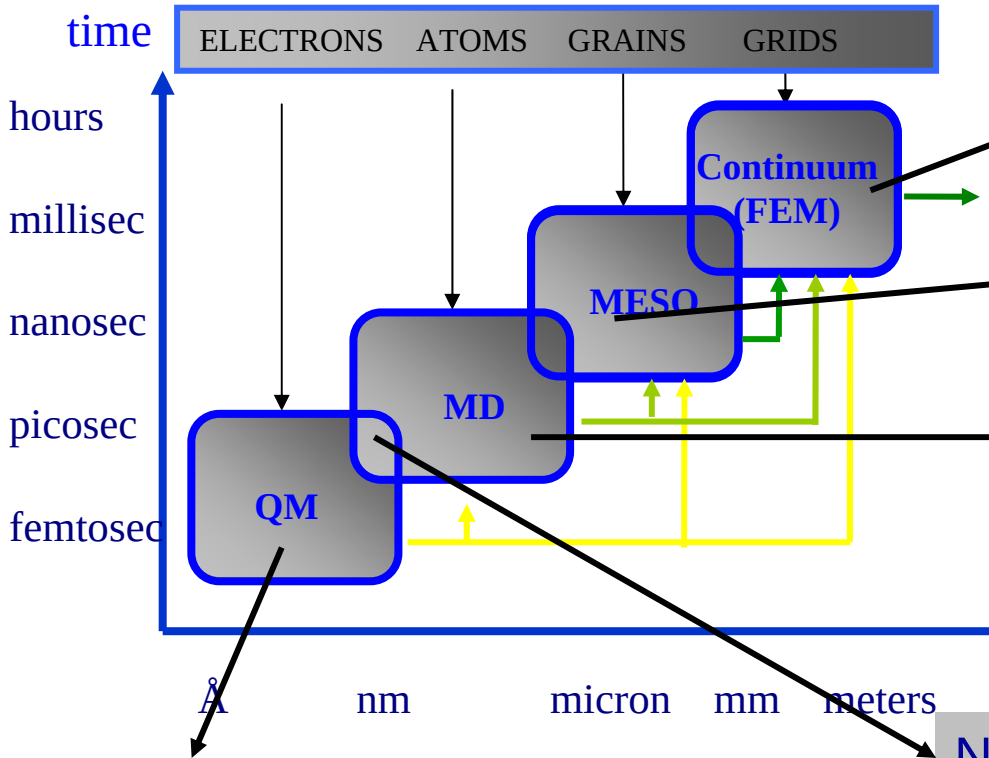
Multiscale Modeling that couples the time and length scales from electrons and atoms to manufacturing

Essential Tools for Theory and computation
Multiscale 1st Principles Design of Materials

Base simulations of large scale systems on First Principles (QM)

Allows Design of new materials and drugs (predict hard to measure properties)

Must connect QM to Design through an overlapping hierarchy of methods



simulations real devices and full cell (systems biology)

Micromechanical modeling
Protein clusters

Deformation and Failure
Protein Structure and Function

New generation reactive force fields based purely on first principles
For metals, oxides, organics.
Describes: chemistry,charge transfer, etc.

Accurate calculations for bulk phases and molecules (EOS, bond dissociation)

Chemical Reactions (P-450 oxidation)

Method Developments at MSC Relevant for Nanotechnology

Quantum Mechanics
- **Solvation (**Poisson-Boltzmann**)**
- **Periodic Systems (**Gaussians**)**
- New Functionals DFT (bond breaking)
- **Quantum Monte Carlo methods**
- Time Dependent DFT (optical spectra)

Force Fields
- **Polarizable, Charge Transfer**
- **Describe Chemical Reactions**
- **Describe Phase Transitions**
- **Mixed Metal, Ceramic, Polymer**

MesoScale Dynamics
- **Coarse Grained FF**
- Kinetic Monte Carlo (Gas Diffusion)
- Hybrid MD and Meso Dynamics
- Tribology

Utilization:
- **Integrated,** Python-based

Molecular Dynamics
- **Non-Equilibrium Dynamics**
  - Viscosity, rheology
  - Thermal Conductivity
- **Solvation Forces (continuum Solv)**
  - surface tension, contact angles
- **Hybrid QM/MD**
- **Plasticity**
  - Formation Twins, Dislocations
  - Crack Initiation
- **Interfacial Energies**
- **Reaction Kinetics**
- **Free energies**

Biological Predictions
- **MembStruck: structure GPCR proteins**
- **HierDock: Binding Site/Energy Ligands**
- **STRUCTFAST: Homology Methods**

Process Simulation
- Vapor-Liquid Equilibria

This provides an idea of where improvements are being made in multiscale simulation methodology to allow new applications

Applications Focus at the MSC/Caltech

NANOSYSTEMS: **Nanoelectronics, Devices** based on **Carbon Nanotubes DNA**
BIOTECHNOLGY: **Membrane Proteins (GPCR), non-natural Amino Acids, Pharma (VLS)**
POLYMERS: **PEM (Nafion), Dendrimers, Gas diffusion, Surface Tension, Biobased**
CATALYSTS: **Methane Activation, Selective Oxidation, ElectroCat (O_2), Polar Olefins**
SEMICONDUCTORS: **Dielectric Breakdown, $Si/SiO_2/Si_3N_4$ interfaces, B diffusion**
CERAMICS: **Ferroelectrics, Zeolites, Exfoliation Clays**
METAL ALLOYS: Glass Formation, Plasticity (dislocations, crack propagation, spall)
ENVIRONMENTAL: **Dendrimers for Selective Encapsulation, Humic acid**
INDUSTRIAL APPLICATIONS (GM-GAPC, ChevronTexaco, GM-R&D, Asahi Kasei, Toray)

- **Polymers: Gas Diffusion, Surface Tension Modification, Water solubility**
  Polymerization Catalysts for Polar Monomers
- **Catalysts: CH_4 activation, Alkylation phenols, zeolites (Acid sites/templates)**
- **Semiconductors: Dielectric Breakdown nanometer oxides, nitrides, B Diffusion in Si**
- **Automobile Engines: Wear Inhibitors (iron and aluminum based engines)**
- **Oil Pipelines: Inhibitors for Corrosion , Scale, Wax; Hydrates, Demulsifiers**
- **Oil Fields: Surfactants for low water/oil interface energy, Basin models**
- **Ceramics: Bragg Reflection Gratings**
- **Catalysts: ammoxidation of propane**
- **Fuel Cells: H_2 Storage, Polymer Electrolyte Membranes, Electrocatalysis**

This provides an idea of the breadth of applications accessible with the emerging multiscale simulation technologies

Stimulation toward solving impossible problems
Collaborations with Industry

- **GM advanced propulsion: Fuel Cells** (store H_2, membrane, cathode)
- Chevron Corporation: **CH_4 to CH_3OH, Alkylation, Wax Inhibition/oil pipeline**
- General Motors - **Wear inhibition in Aluminum engines**
- **Seiko-Epson: Dielectric Breakdown in nm oxide films, TED** (B/Si)
- Asahi Kasei: Ammoxidation **Catalysis, polymer properties**
- **Berlex Biopharma: Structures and Function of CCR1 and CCR5 (GPCRs)**
- **Aventis Pharma: Structures and Function of GPCRs**

Previous

- Asahi Glass: Fluorinated Polymers and Ceramics
- Avery-Dennison: Nanocomposites for computer screens Adhesives, Catalysis
- BP Amoco: Heterogeneous Catalysis (alkanes to chemicals, EO)
- Dow Chemical: Microstructure copolymers, Catalysis polymerize polar olefins
- Exxon Corporation: Catalysis (Reforming to obtain High cetane diesel fuel)
- Hughes Satellites/Raytheon: Carbon Based MEMS
- Hughes Research Labs: Hg Compounds for HgCdTe from MOMBE
- **Kellogg: Carbohydrates/sugars** (corn flakes) **Structures, water content**
- MMM: Surface Tension and structure of **polymers**
- **Nippon Steel: CO + H_2 to CH_3OH over metal catalysts**
- Owens-Corning: Fiberglas (coupling of matrix to fiber)
- Saudi Aramco: Demulsifiers, Asphaltenes

Each project (3 Years) supports full time postdoc and part of a senior scientist

This provides an idea of those applications being funded by industry that use multiscale simulation technologies

Nanotechnology applications demand many scales to combined seamlessly

To do this we are developing the Computational Materials Design Facility

Create an integrated, component-oriented toolset combining existing simulation software technology in novel ways

Develop multi-scale techniques that automatically span length and time scales, in a grid-aware environment

Rapid prototyping and development

Quickly assay materials properties simulation results

Rank the success of the simulations, and

Visualize the most promising candidates

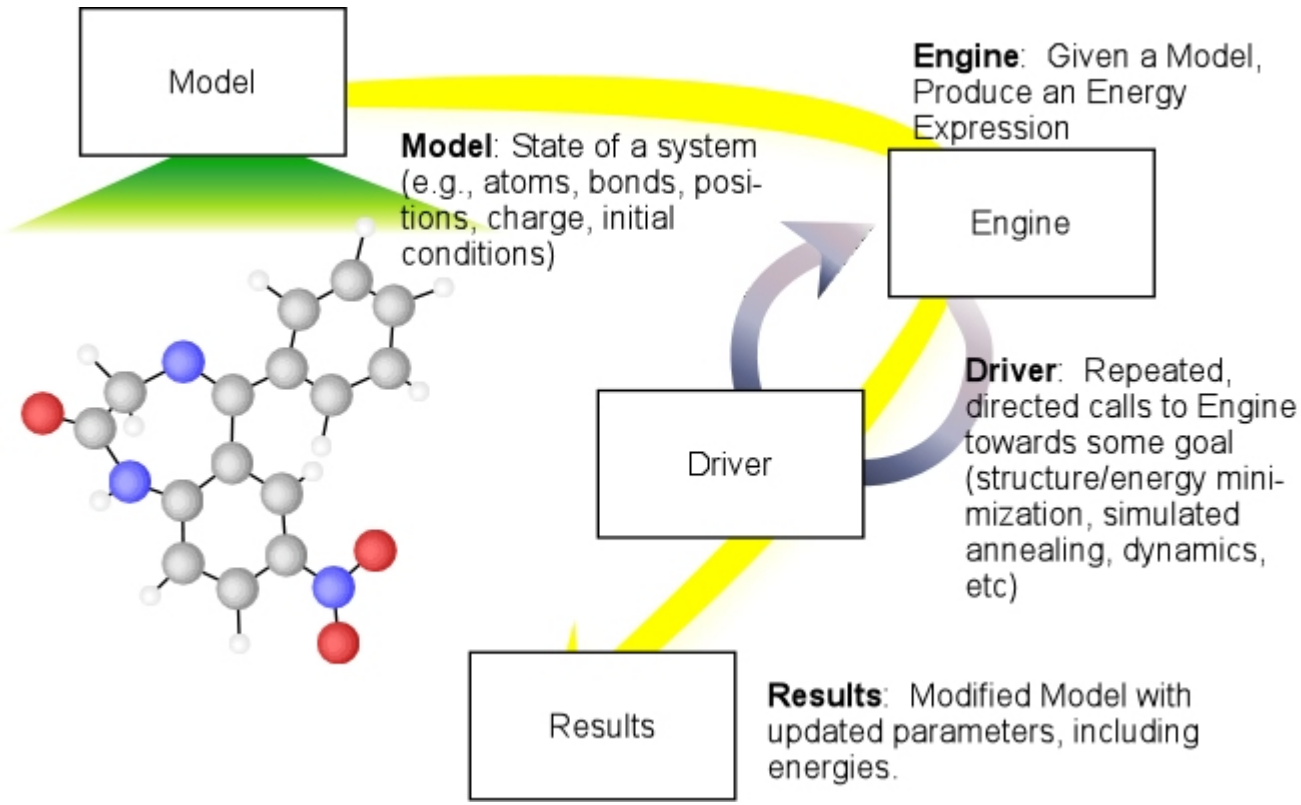
Funded by DARPA (Carey Schwartz)

CMDF: Software Architecture Component Structures

Engine: abstract interface to existing computational code can be command line or library/function call

Driver: abstract task-oriented methodology: make the engine 'do' something; e.g., traversing length scales

Model: a 'state' variable including structure, energy, phase, grain interface, etc



CMDF software framework

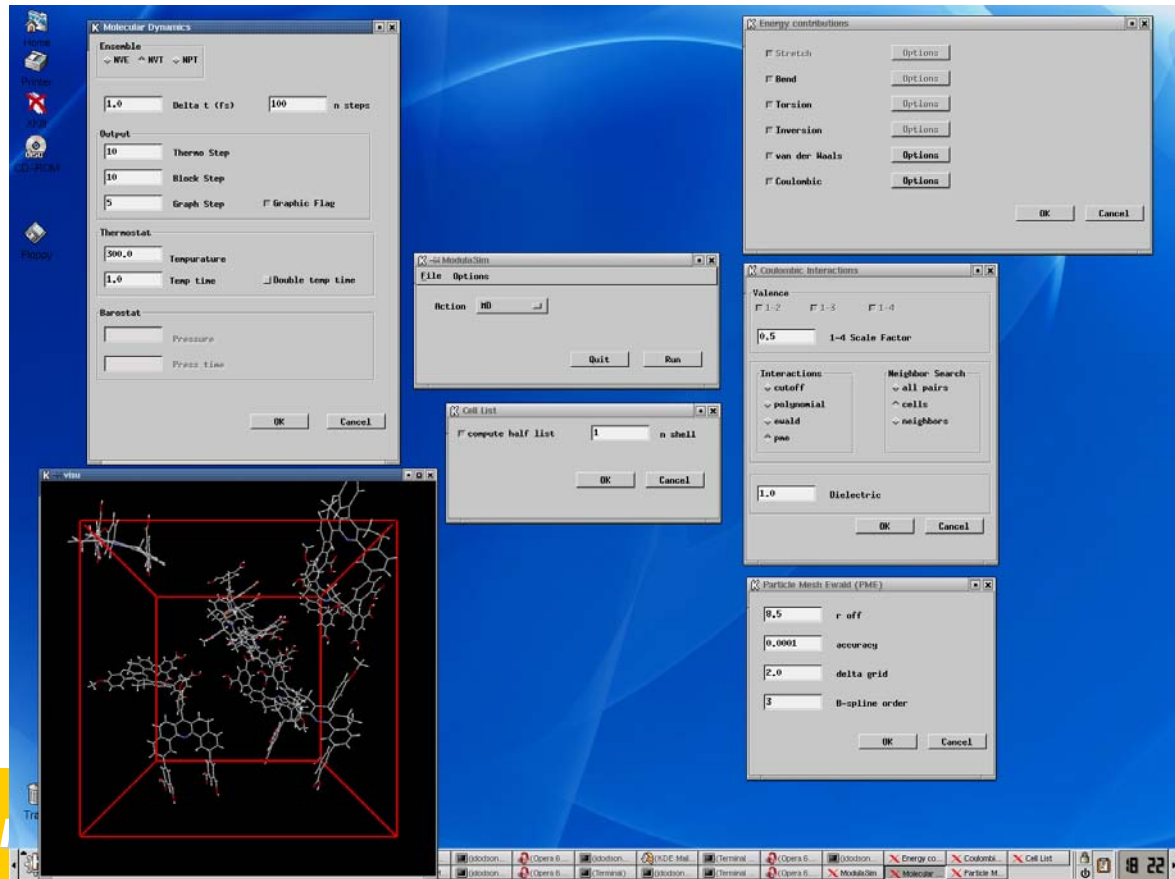
- **Developing methods**
- Software to **organize** and **automate** multiscale simulations
- Capture, store, manipulate simulation results in a **scale-agnostic** manner
- Create a **framework** and **toolkit** to develop multi-scale applications
- **Provide** that framework/toolkit and methods to the community

Developed 'ModSim', MD code with modularity and ease of development

Using SWIG, we have created a python interface to the main programming routines, Swig generates 'glue' between library functions in c/c++ and common scripting languages (python, perl, tcl, ruby, etc), Nearly automatic generation of interfaces

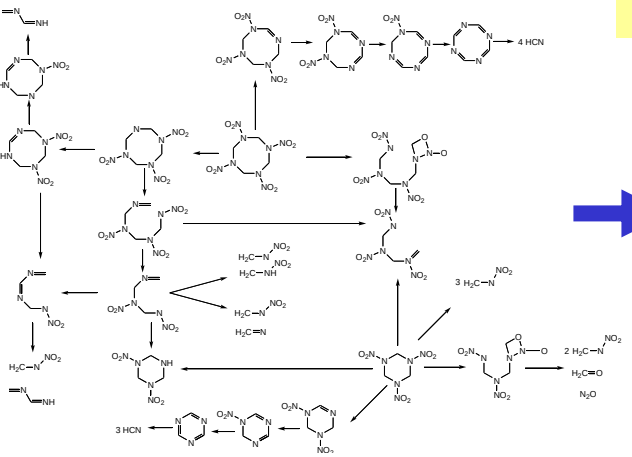
Replaced the 'c' main loop of MPSim with a python loop, then as a further step recoded the c MD loop and force summation step in python with **no noticeable overhead** (<< 1%)

Allows easy GUI development, more control over program, easy development

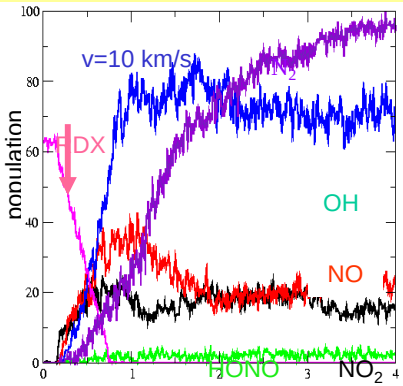


CMDF Full-physics multi-scale modeling

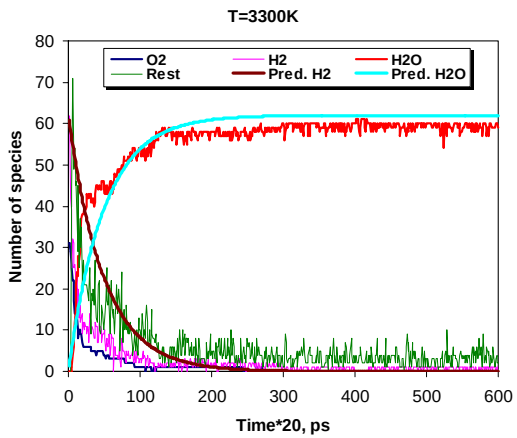
Energetic materials



Detailed QM



ReaxFF MD

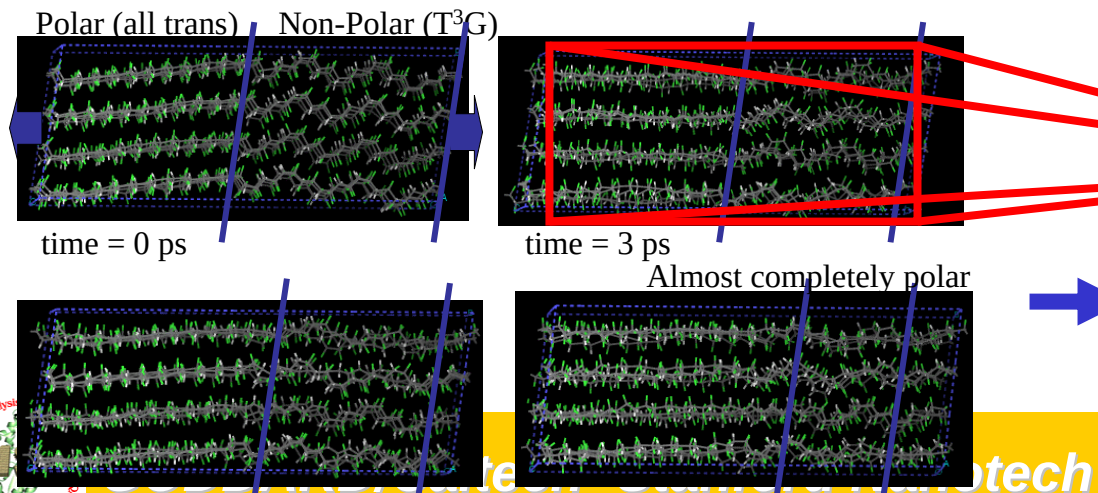


Continuum (Cantera)

Ferroelectric polymers

Atomistic modeling:

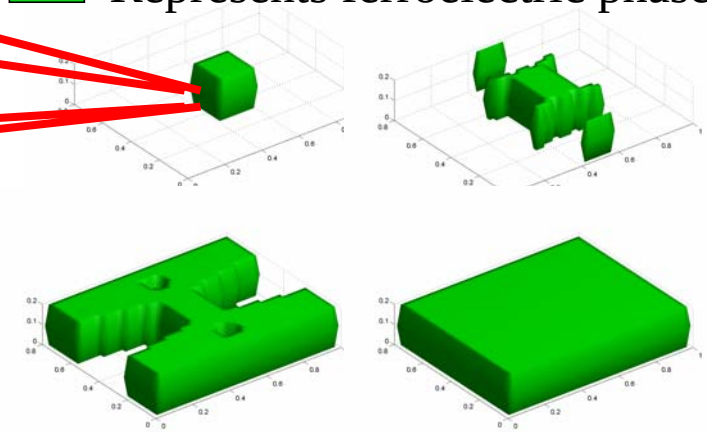
Stress induced phase transformation



Mesoscopic modeling:

Stress induced phase transformation

Represents ferroelectric phase



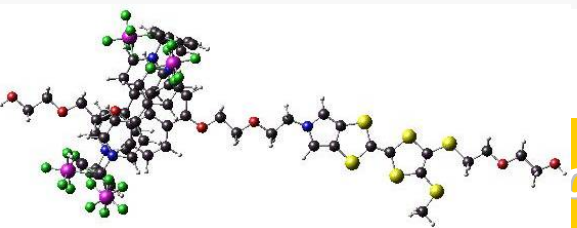
MSC Projects in Nanotechnology

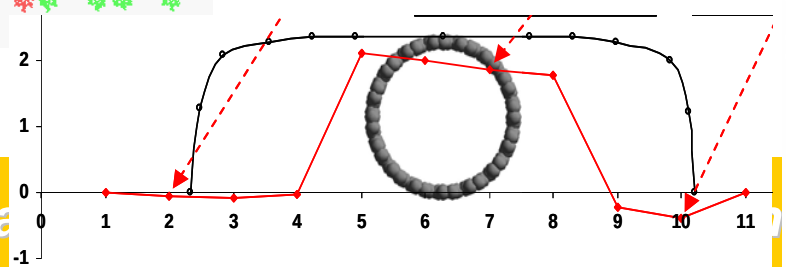
DNA machines: collaboration with Ned Seeman (NYU) and Erik Winfree (CS/Caltech)

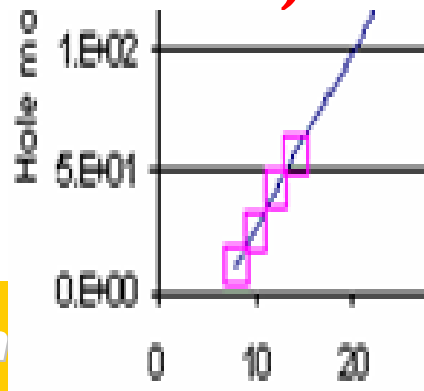
Molecular Switches: collaboration with Fraser Stoddart (UCLA) and Jim Heath (Chem/Caltech)

Molecular electronics: high mobility organics, proton switches

Simulation of AFM Imaging: collaboration with Pat Collier (Chem/Caltech) and Steve Quake (APh/Caltech)

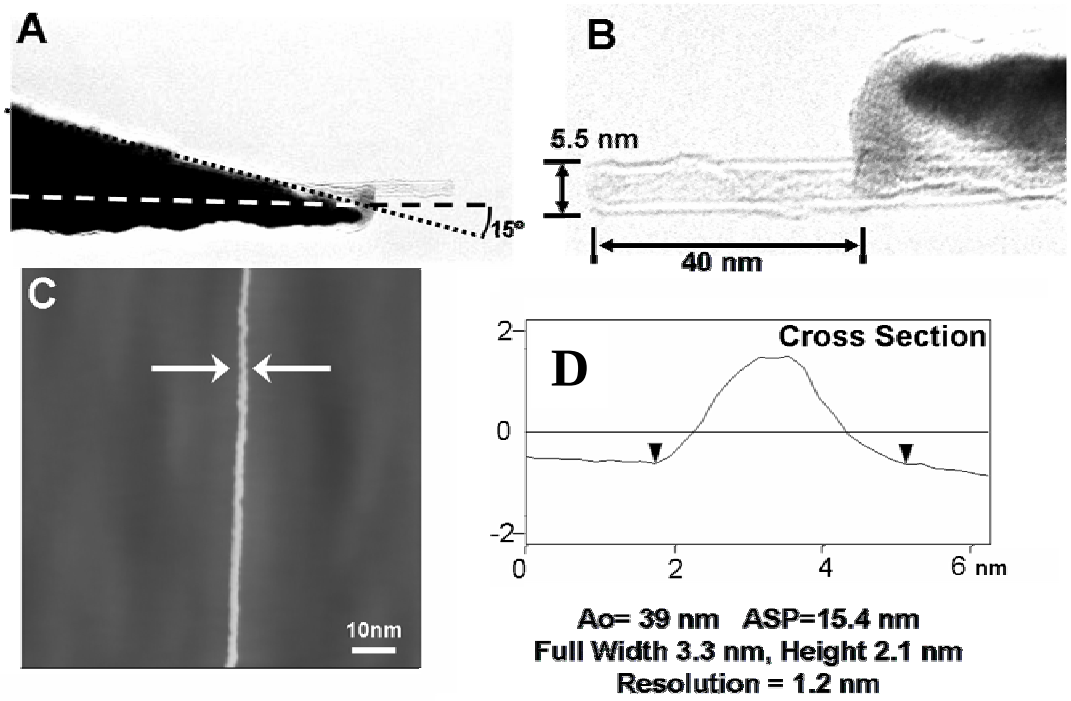






AFM Simulation Methods: MD and AFM Dynamics

Santiago Solares, Ian Shapiro, Maria Jose Esplandiu, Larry Wade, Yuki Matsuda, Stephen Quake,
Pat Collier and William A. Goddard III



Experiments

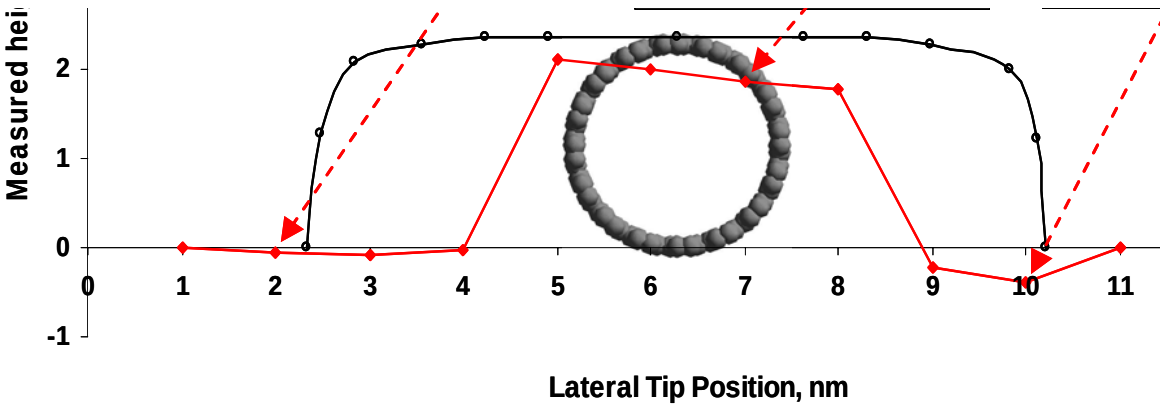
A. TEM image of a SWNT tip attached to Si support tip

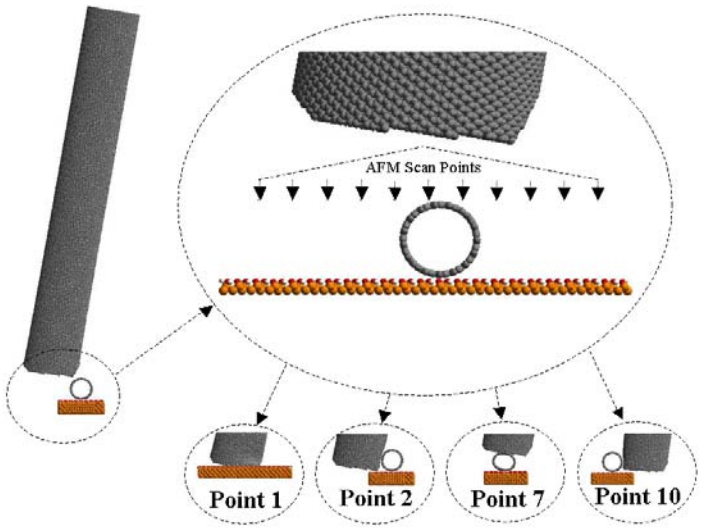
B. Close-up of SWNT tip showing dimensions

C. AFM image of a carbon NT using above probe

D. Cross-section AFM trace at location in figure C

MD Simulation of AFM image





Simulated AFM Scan
Ideal Probe Scan

New Materials for Organic Electronics

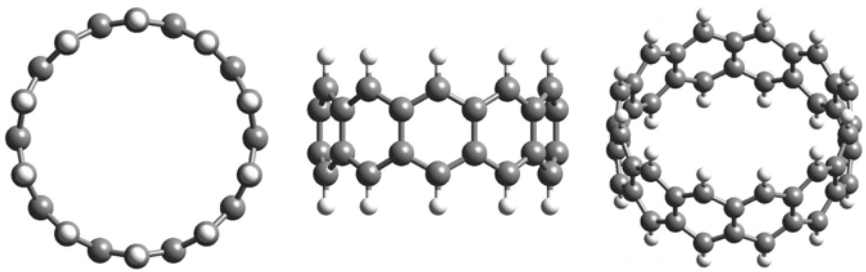
Current material of choice for molecular electronics: Pentacene

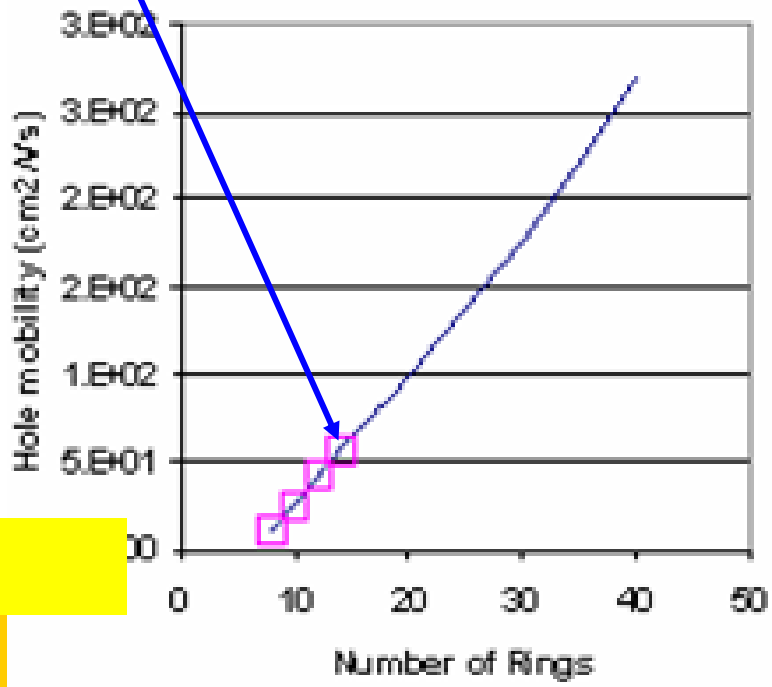
Films lead to hole mobilities of 3 to 7 cm^2/V sec (most accurate ~ 5)

We developed an incoherent transport model and calculate a hole mobility of 6.5 cm^2/Vs for pentacene crystals at 300K. In reasonable agreement with experiment

We find that an alternative packing into a crystal should lead to a hole mobility of 15.2 cm^2/Vs, suggesting that pentacene might still be improved by a factor of ~3.

Considering a variety of alternative materials we find that bracelets of aromatics can lead to hole mobilities of 50 cm^2/Vs or more are possible.





Challenge: to make these at a practical cost

GODDARD/Caltech Stanford Nanotech

Nanoelectronics

Many experimental efforts to make nanoscale electronic devices based on molecules sandwiched between conducting surfaces (e.g., Jim Heath/UCLA-Caltech, Charley Lieber/Harvard, ~~Jan Schön/Lucent~~, Phaedon Avouris/IBM)

This could be most useful. For example a future MEMS-scale device (say 20 microns in size) might have an onboard computer based on nanometer sized elements with built in sensors and logic to respond to local environment without the necessity of communicating to remote computer.

Thus to be useful the nanosized switches need not be as fast as current computer elements (GHz). They could be even as slow as KHz and still be useful.

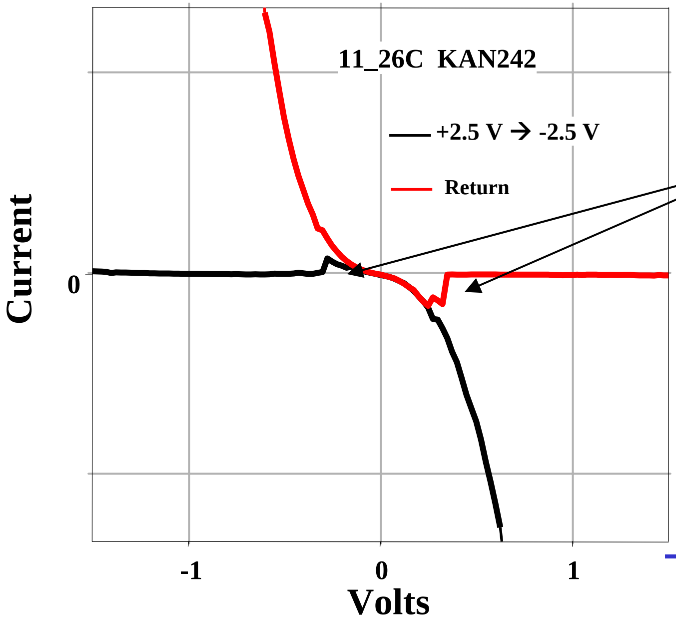
Unfortunately little is known about the atomic-level structure and properties of these nanoelectronics systems, making difficult the design of improved devices.

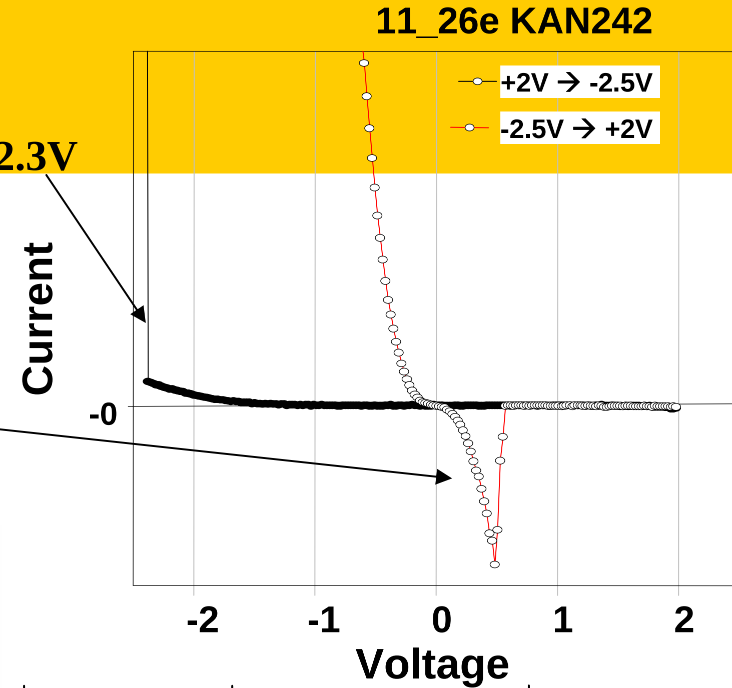
Molecular Switch (Heath & Stoddart)

Fraser Stoddart (UCLA) Jim Heath Caltech)

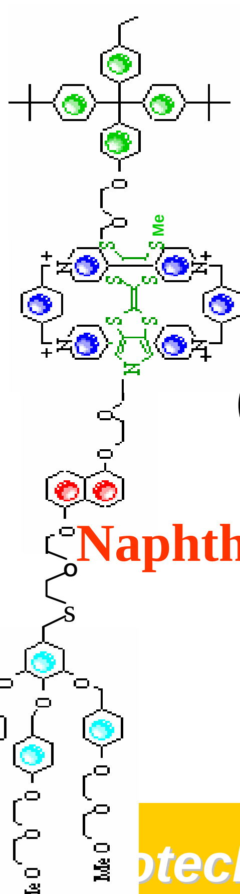
Switch diode orientation at –2.3V

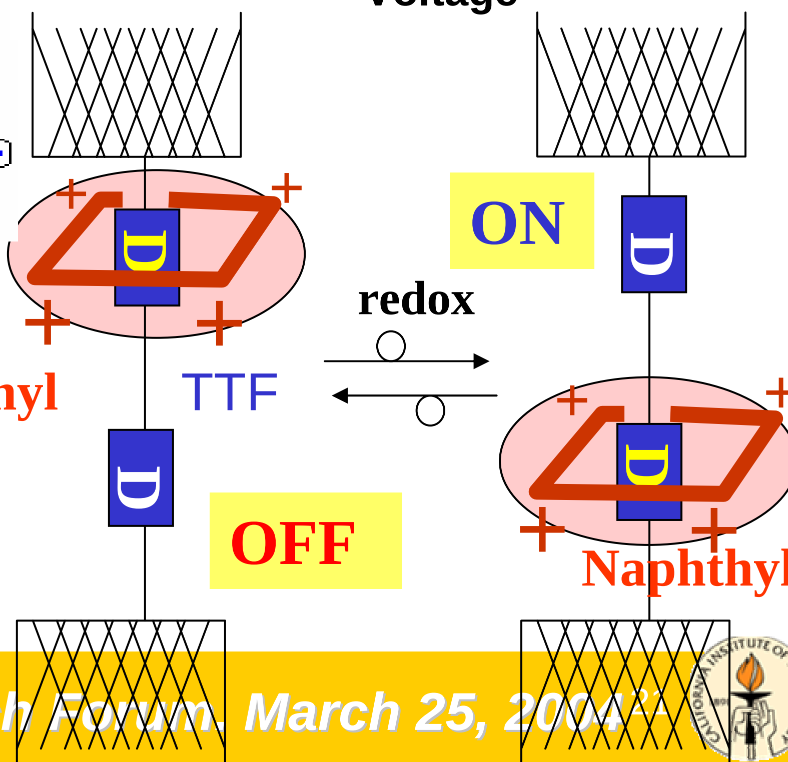
NDR=Acceptor Charging(?)





TTF





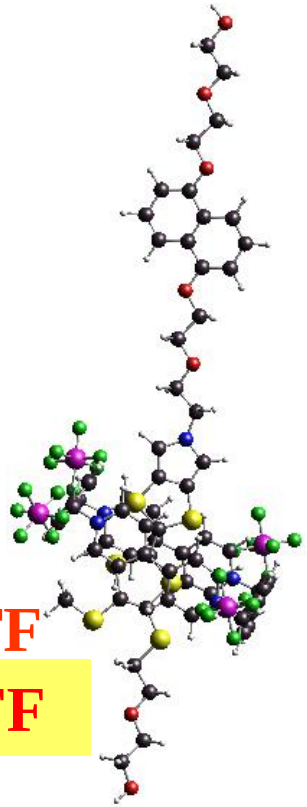
Napthyl and TTF nearly equally good donors

Rotaxane ring binds to TTF > 300K

Rotaxane binds to napthyl > 250K

Assume ring moves when apply external voltage which cause diode to switch.

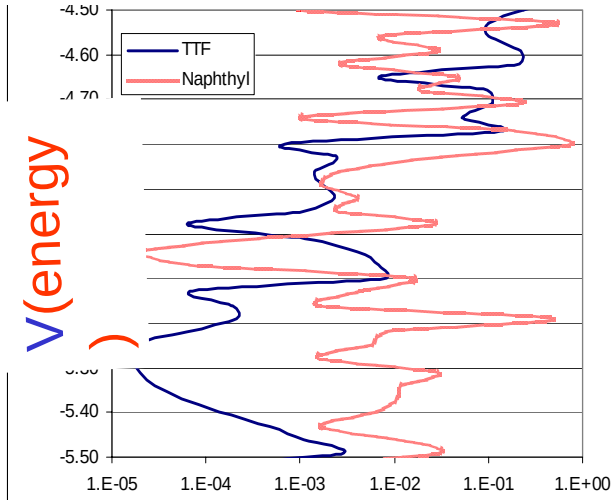
Atomic level simulation of Current/Voltage



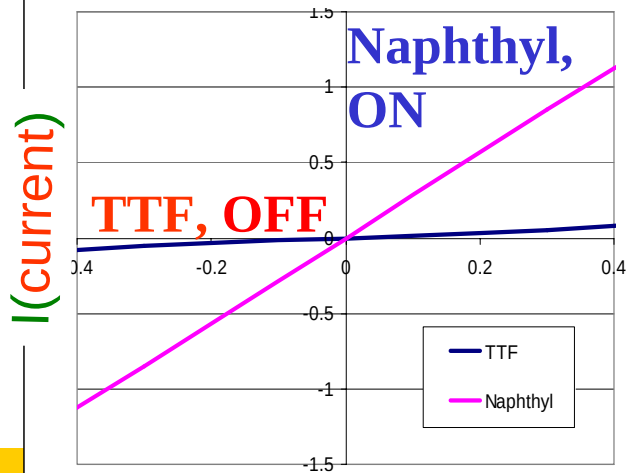
TTF

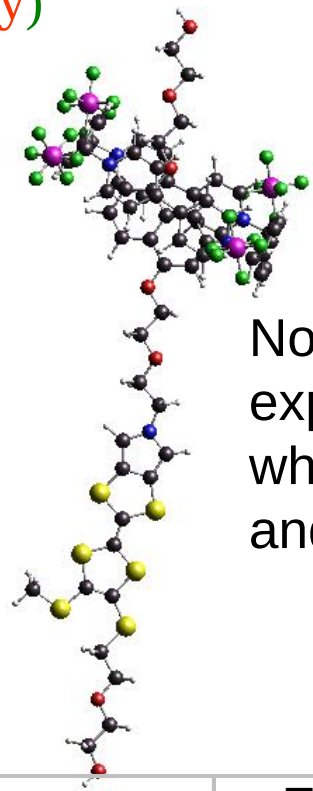
OFF

Predicted I(transmission) -V(energy)



I(transmission)





Naphthyl

ON

Not known experimentally which state is on and which is off

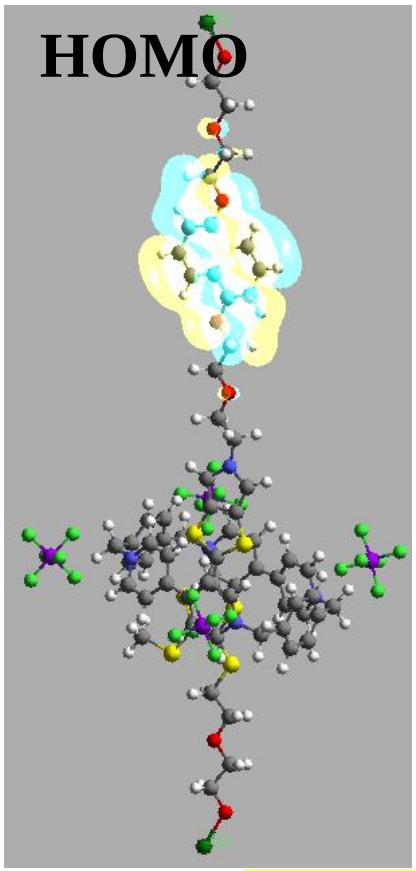
	TTF	Naphthyl
HOMO-1	-6.51	-6.36
HOMO	-5.56	-5.09
LUMO	-5.00	-4.93
LUMO+1	-4.59	-4.85

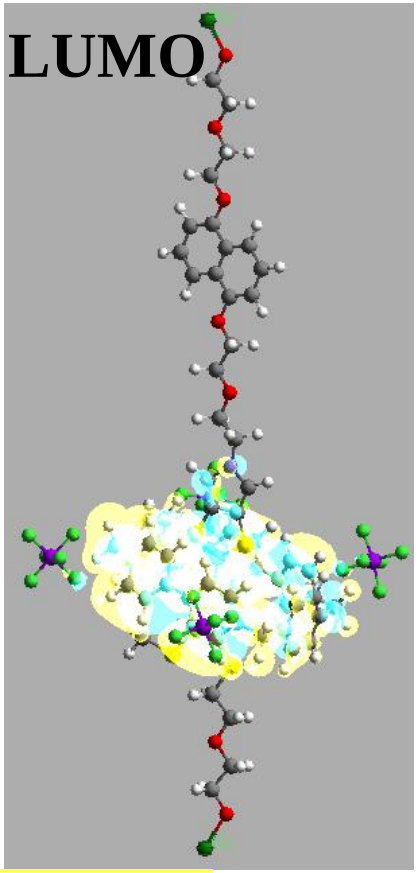
$$H = H_M + \Sigma$$

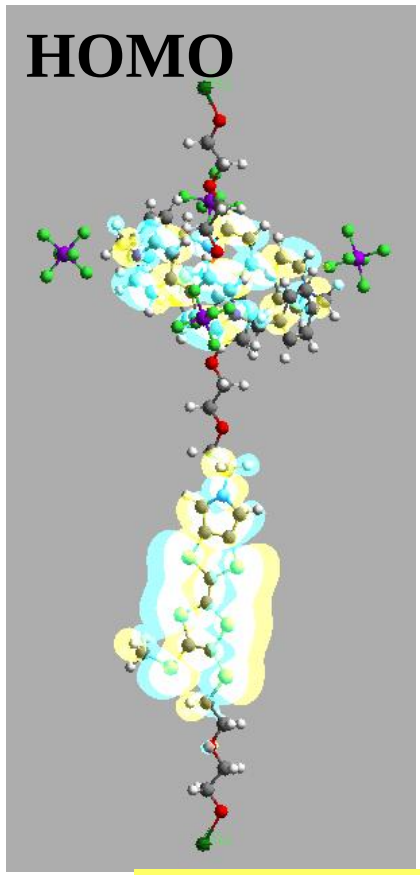
Shapes of Molecular orbitals (MOs)

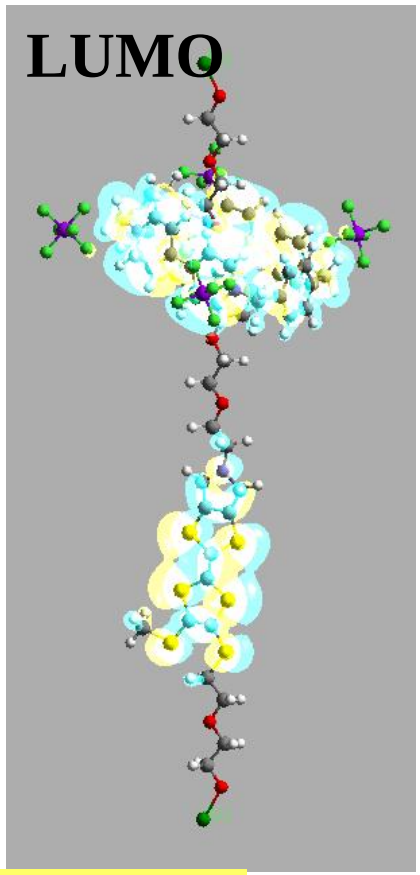
TTF, OFF

Naphthyl, ON







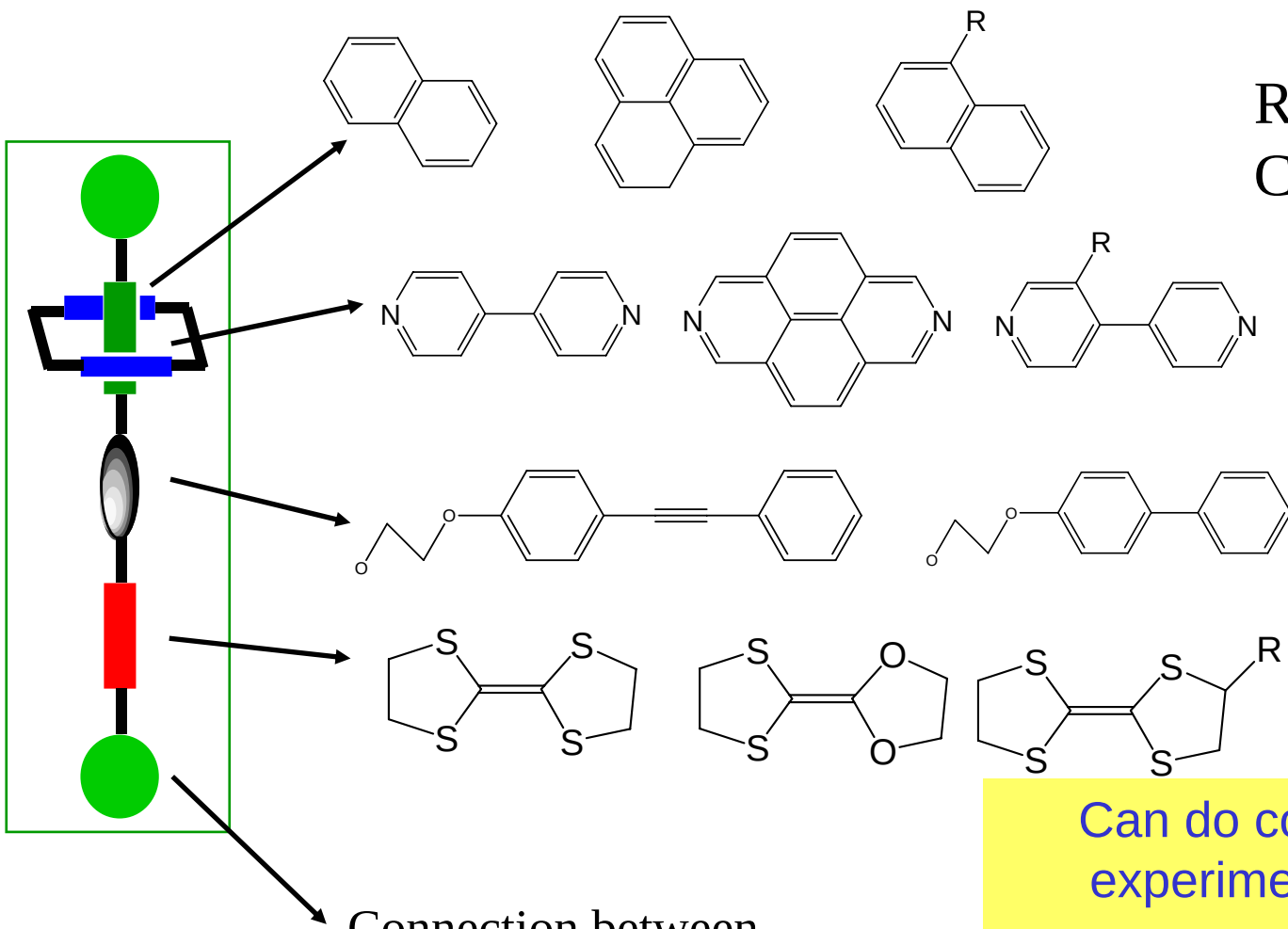


Big gap
not coupled.
~insulating

Nearly degenerate,
thus strongly coupled.
~metallic

Theory provides the underlying mechanism explaining performance, now use for design

Research plan: Rapid Prototyping using theory to optimize molecules for devices



R = NO_2, CN, COOH, OH etc

etc

Connection between molecule tail and electrode

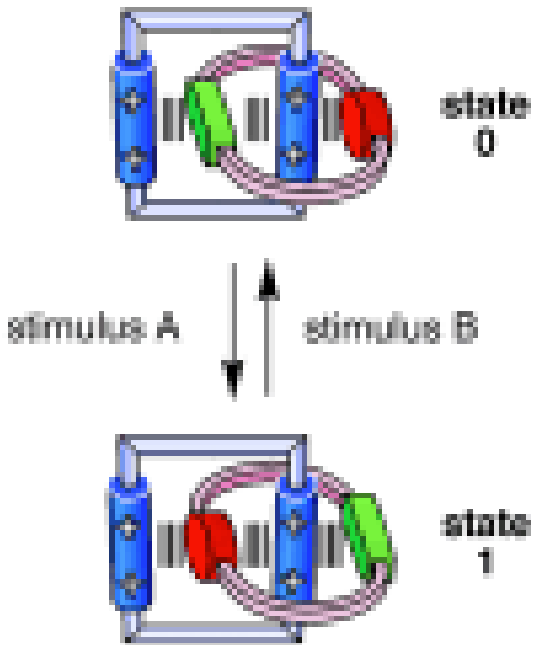
Can do computational experiments in hours

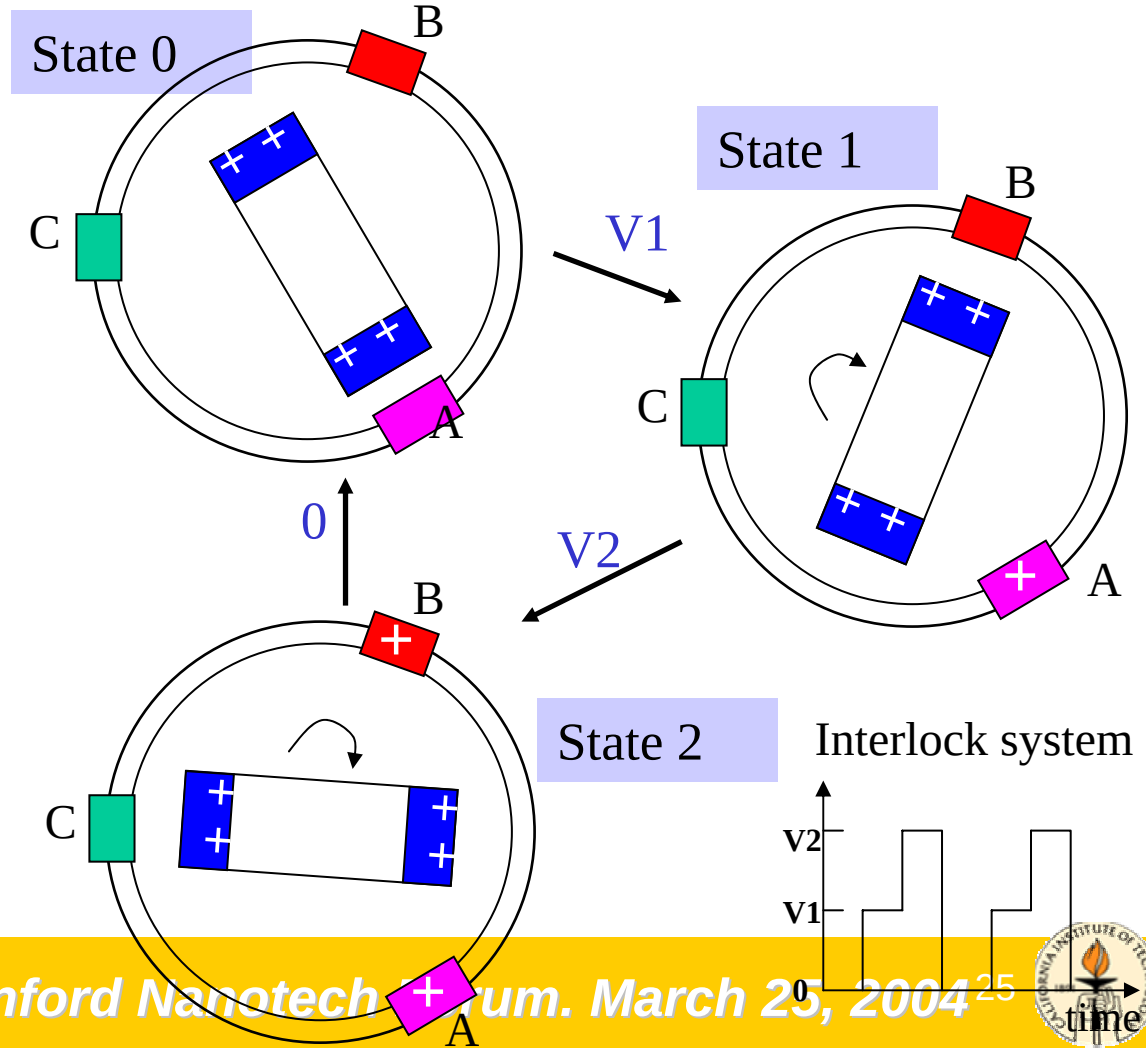
Lab experiments sometimes months

Design of a Rotary nano-motor

Caltech designed a rotary nano-motor using components similar to the UCLA switch. Features:
Three different groups in outer ring with different oxidation potentials, two identical groups in the inner ring.
The oxidation potentials of groups A,B are v1,v2
The inner ring will rotate clockwise

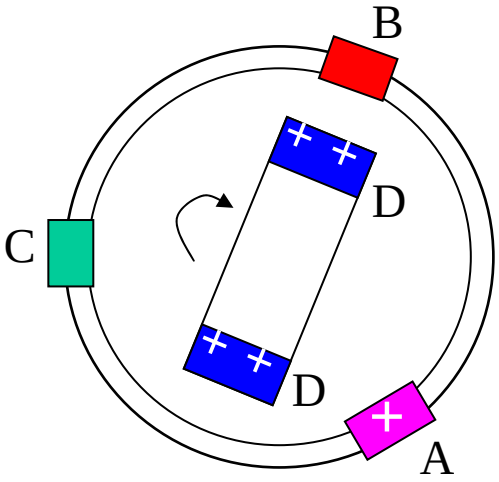
Stoddart (UCLA) has demonstrated a 2-state molecule but cannot control the direction of movement. Thus cannot make a motor

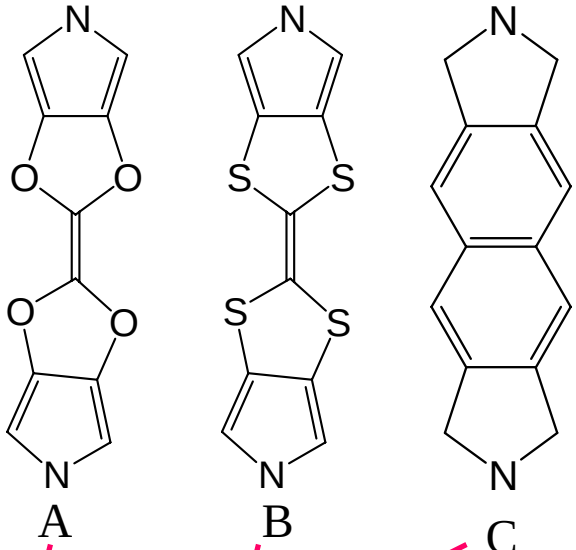


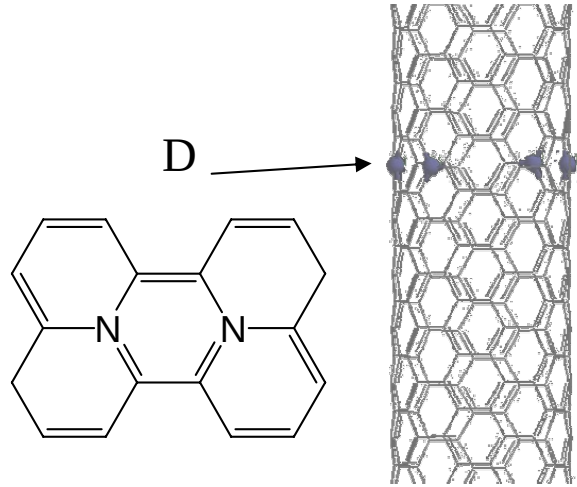


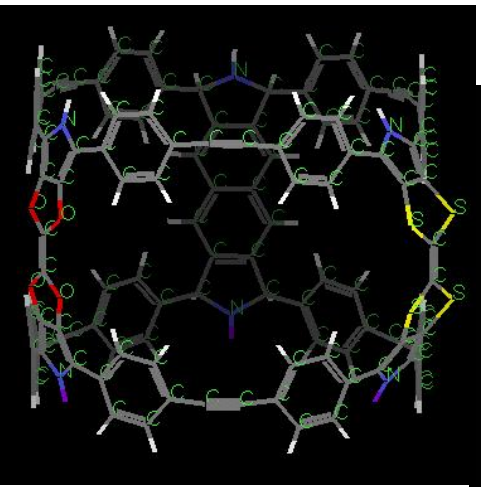
Under testing (theory)

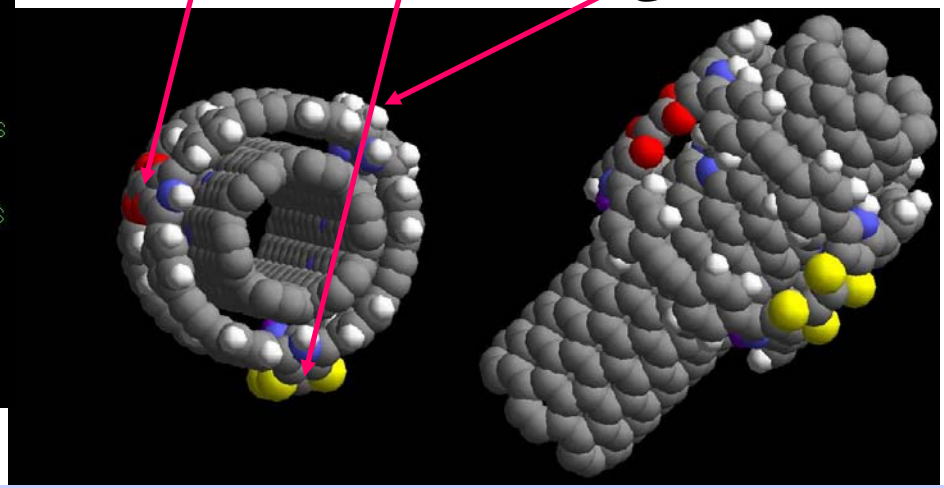
key design issues
choosing A B C D groups

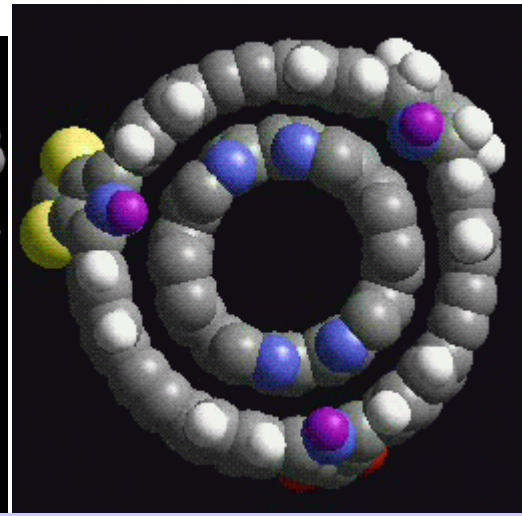






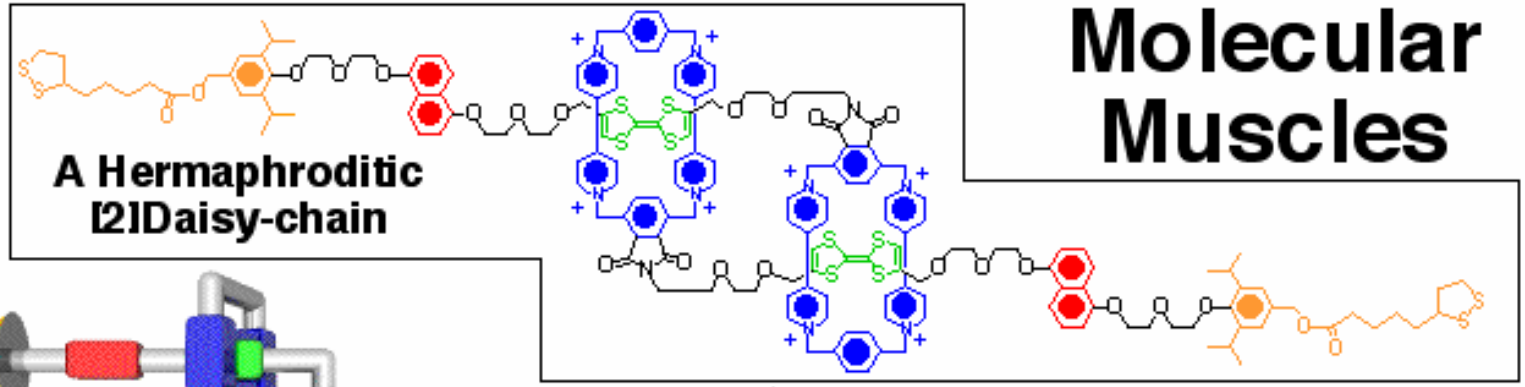


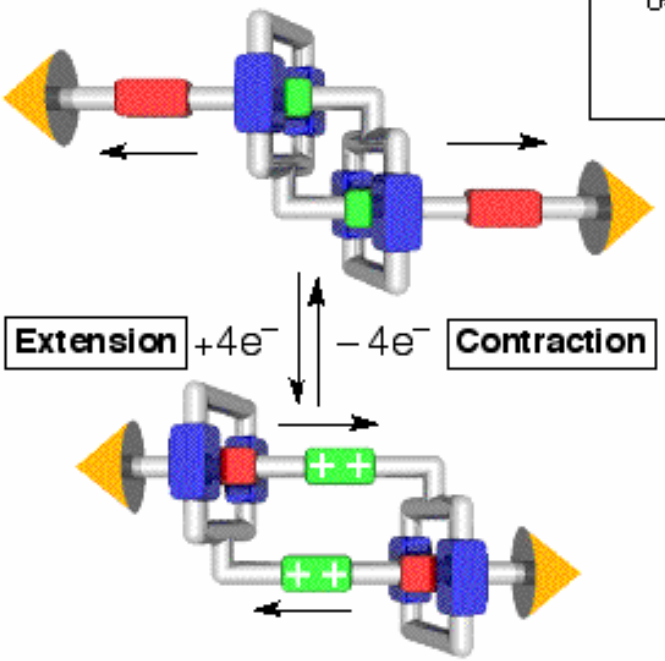


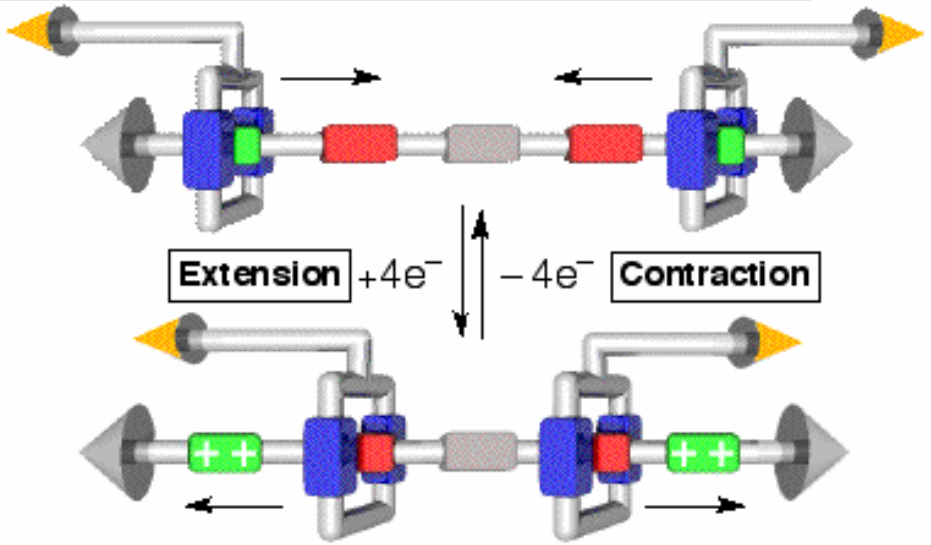


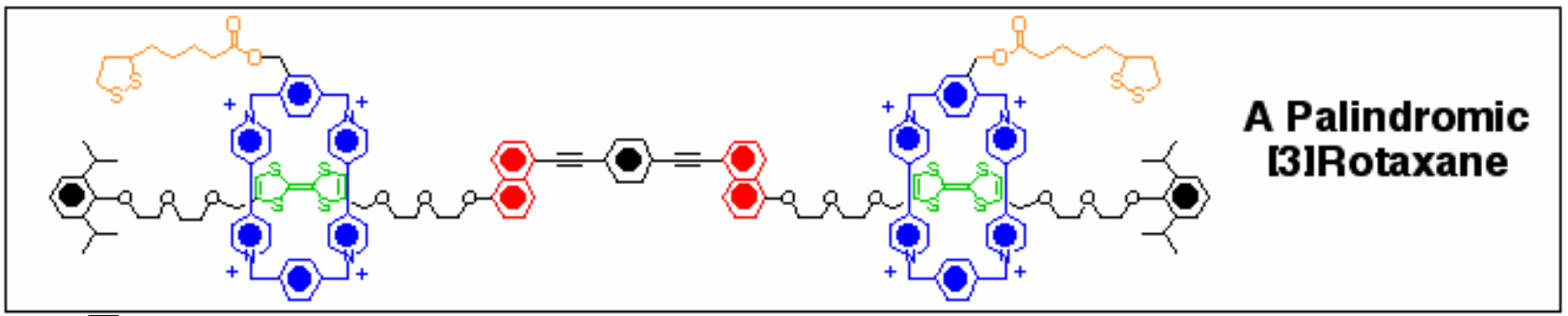
The calculations will determine the maximum switching speed and resonant frequencies to be avoided. Also the theory will be used to determine the right components for convenient redox potentials

Molecular Muscles







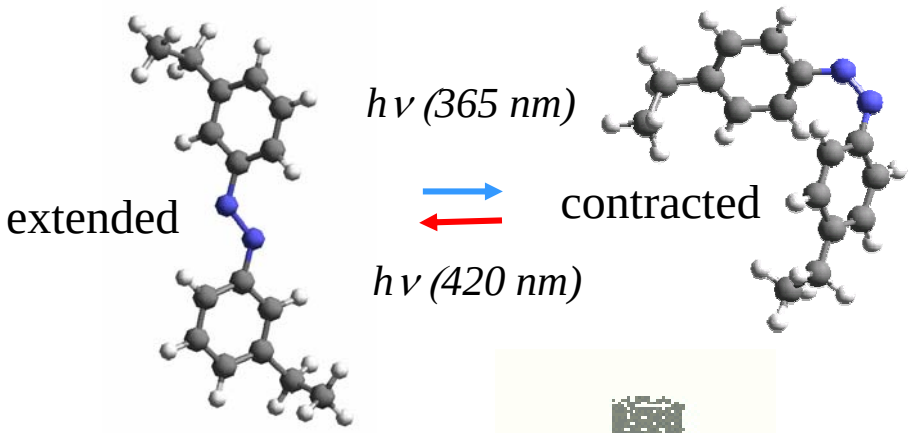


Exper. Ho — Montemagno — Stoddart — Tai — Zhang UCLA

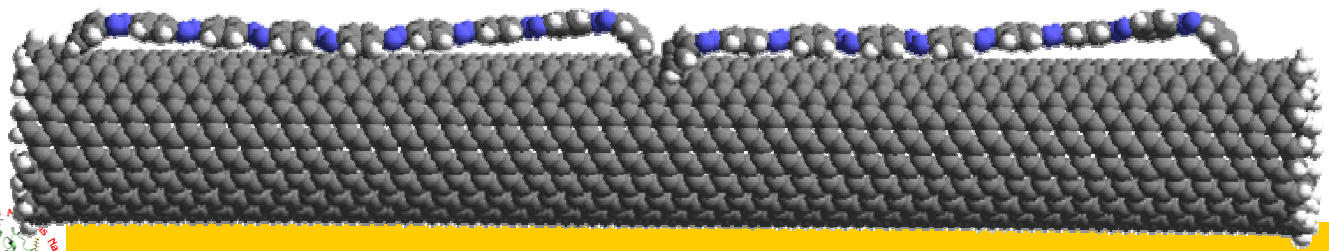
Theory: Goddard, Caltech

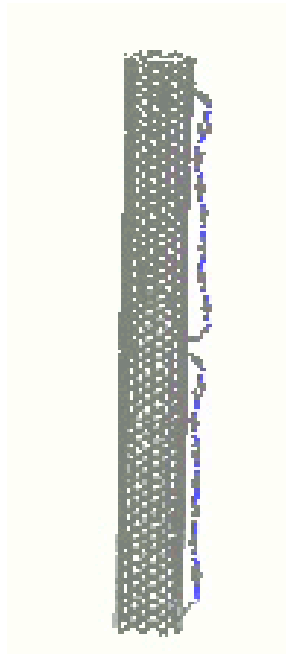
Opto-mechanical Muscles

- **Azobenzene monomer response to light**
- 365 nm trans ⟶ cis
- 420 nm cis ⟶ trans
- Tension of a single strand ~ 205 pN
- Length change per monomer ~ 0.25 nm
- Not to exceed 50 nm in length for good efficiency in Quantum yield



- **Determination of mechanical properties**
- **Integration into NEMS**





So far have talked about software tools

New tools for experimental synthesis and characterization are also critical to timely advances in nanotechnology.

I will summarize just the one case I have been involved in.

Traditional dry etching techniques use ions to blast of the Si and other atoms on a surface. This leads to significant surface damage and rough surfaces. We have been working on ways to use electrons to tickle off the surface atoms (chemisrty, putting the electrons in antibonding orbitals to break the bonds) rahter than physically blasting the atoms off with ions.

The intellectual leadership has been due to Pat Gillis who has taken a leave from UCLA to commercial his inventions.

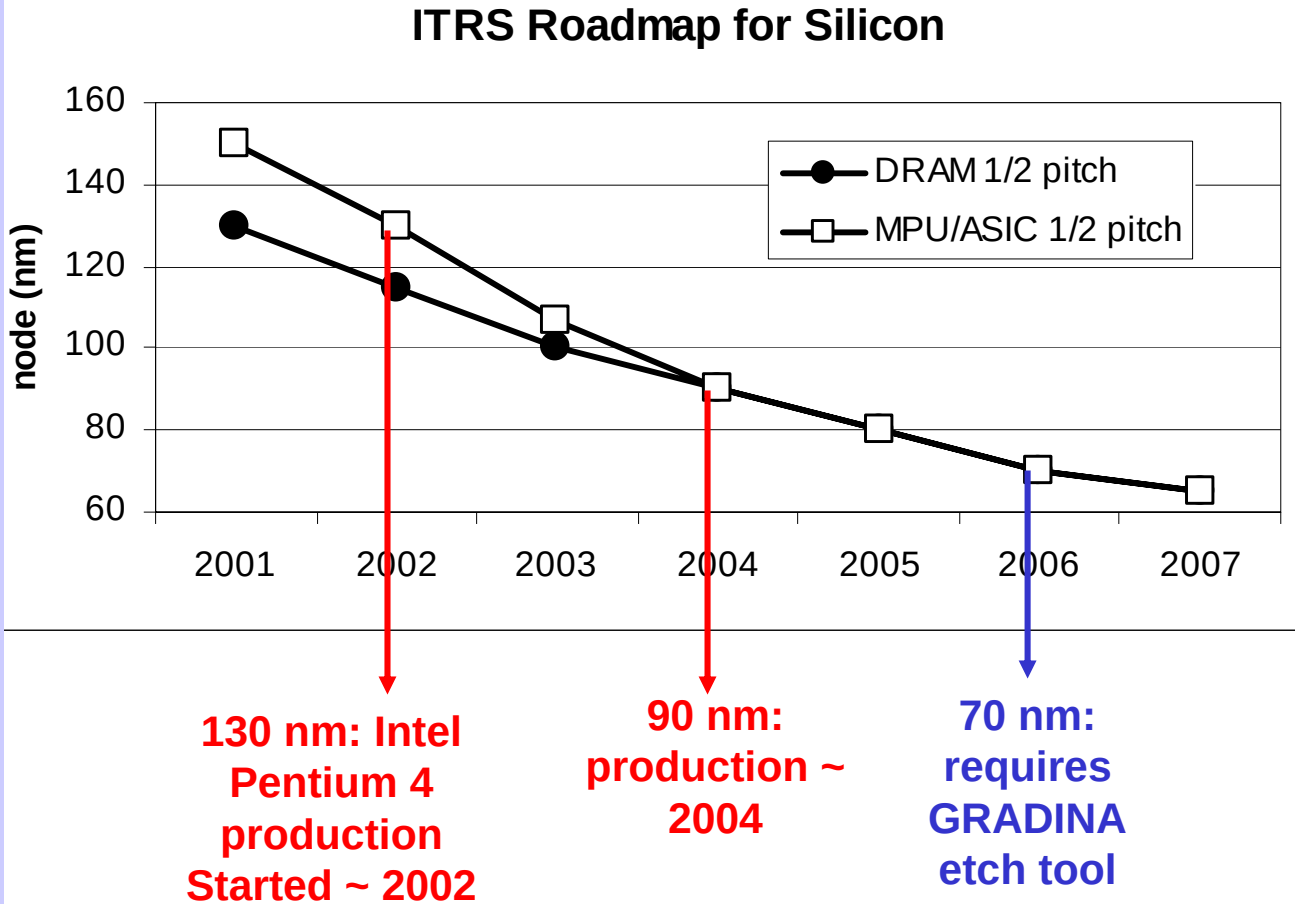
The Gradina Tool for Nanoelectronics

Dry etching techniques using ions create significant surface damage and at 90nm this damage creates severe quality problems.

These techniques probably cannot be extended to 70 nm.

Gradina incorporates the revolutionary new low energy enhanced etching (LEEE) technology invented by Pat Gillis (UCLA). This has demonstrated damage free etching down to 20 nm with etching rates similar to ions

MOORE'S LAW Schedule for Si Devices

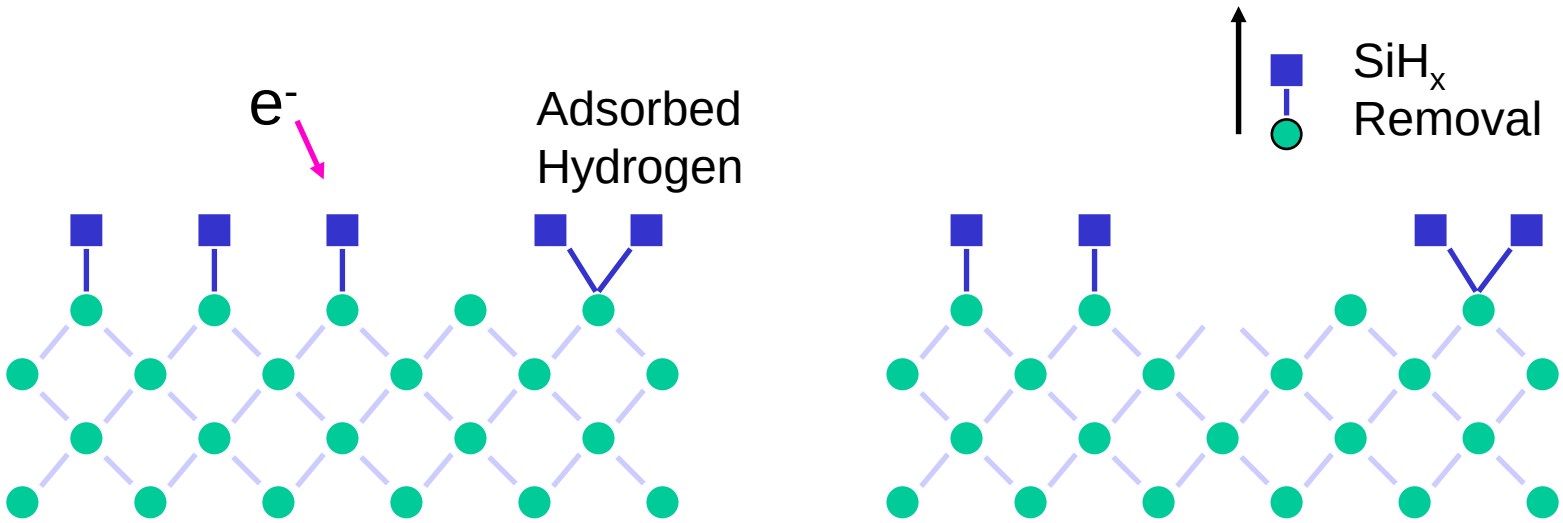


Gradina has demonstrated damage free 20 nm structures….

Low Energy Electron Enhanced Etching (LE4):

Gillis, Chamberlain, Clemons, JVST. ***B10,*** *2927 (1992)*

- Use Low Energy Electrons from Gas Discharge to *Chemically* etch the atoms from the surface (contrast with Ion Etching that *Physically* knocks off the atoms)
- Avoids damage by eliminating ion bombardment
- Proceeds via electronic excitations at surface
- Surface atoms removed by reaction product desorption
- Driven by material specific energy thresholds



PROBLEMS WITH ION-ENHANCED ETCHING

Damage Permeates Mesa

Poor Interfaces in Recesses

Solution: Design a Damage-Free Etch Process

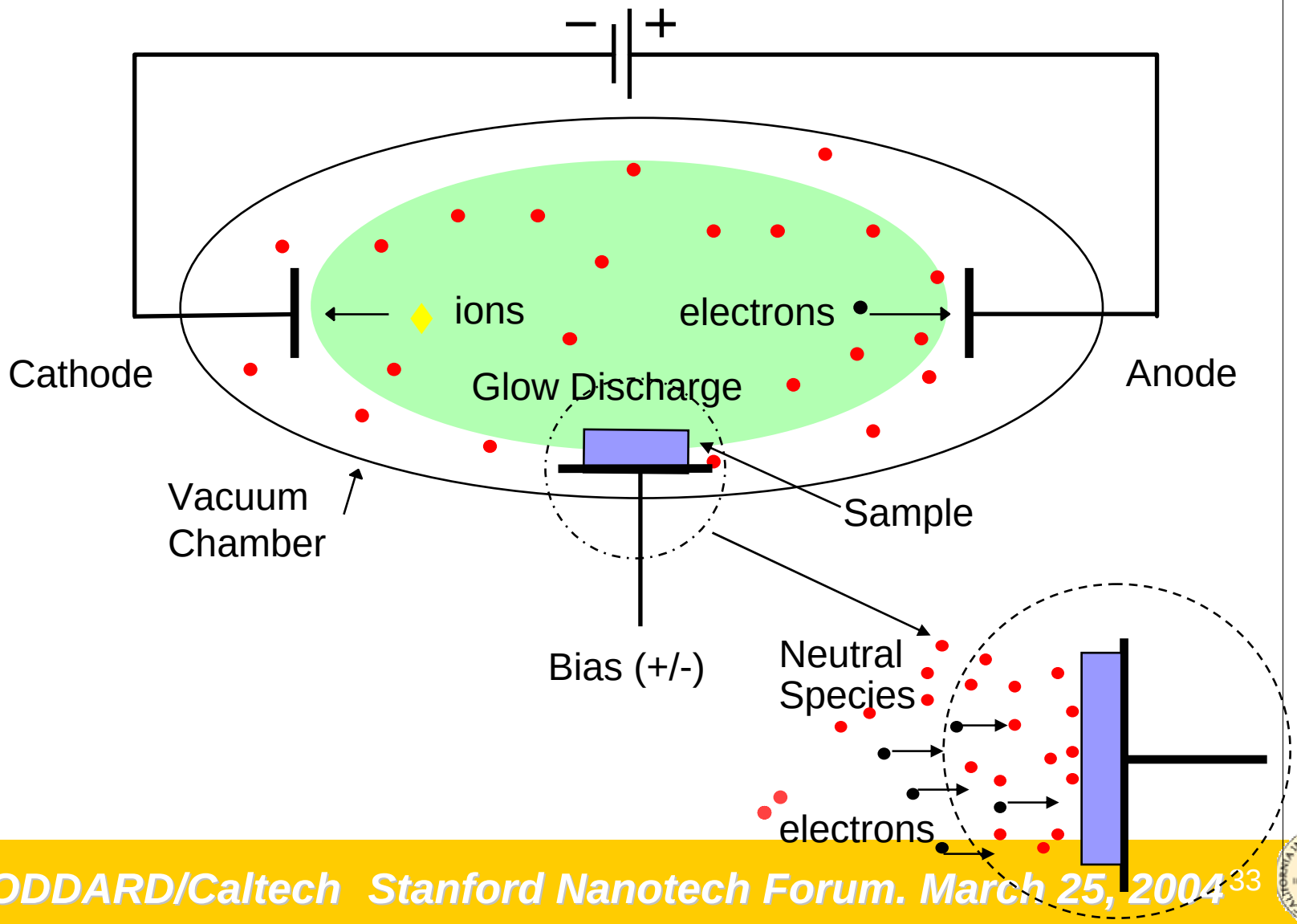
- Avoid ion-enhanced chemistry to eliminate lattice damage
- Use low-energy electron enhanced chemistry to achieve anisotropy

Low-Energy Electron Enhanced Etching (LE4)

- Electron flux at energy below 100 eV
- Reactant flux at thermal velocities

Etching in a DC Plasma

Gillis, Choutov, Martin, et al. Appl. Phys. Lett. 66, 2475 (1995)

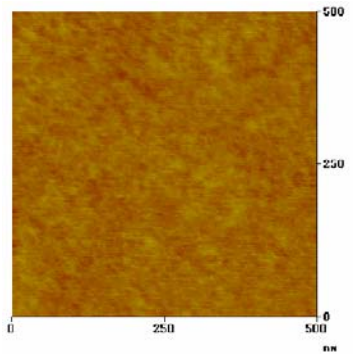


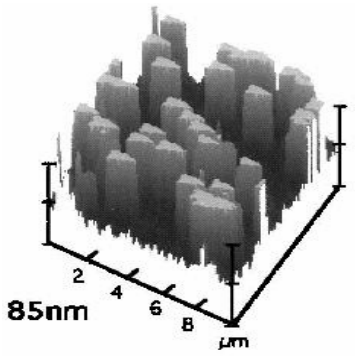
Gradina™ Competitive Advantages for GaN & Other Compound Semiconductors

(High Yield) x (High Throughput) = High Margins

PRODUCES HIGH YIELD

RMS Surface Roughness





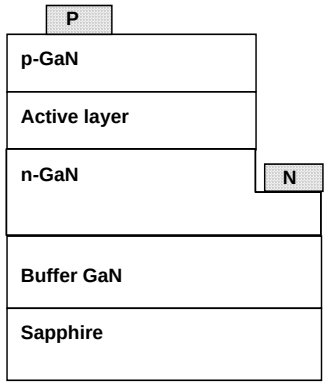
LE4: 0.25 nm ECR: 85.0 nm

LE4 is 340x Smoother

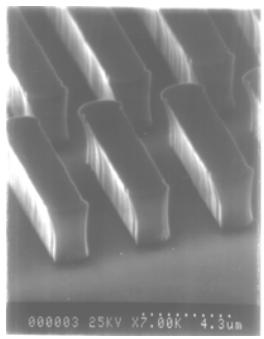
INCREASES THROUGHPUT

Etch Rate

GaN LED/LD Structure



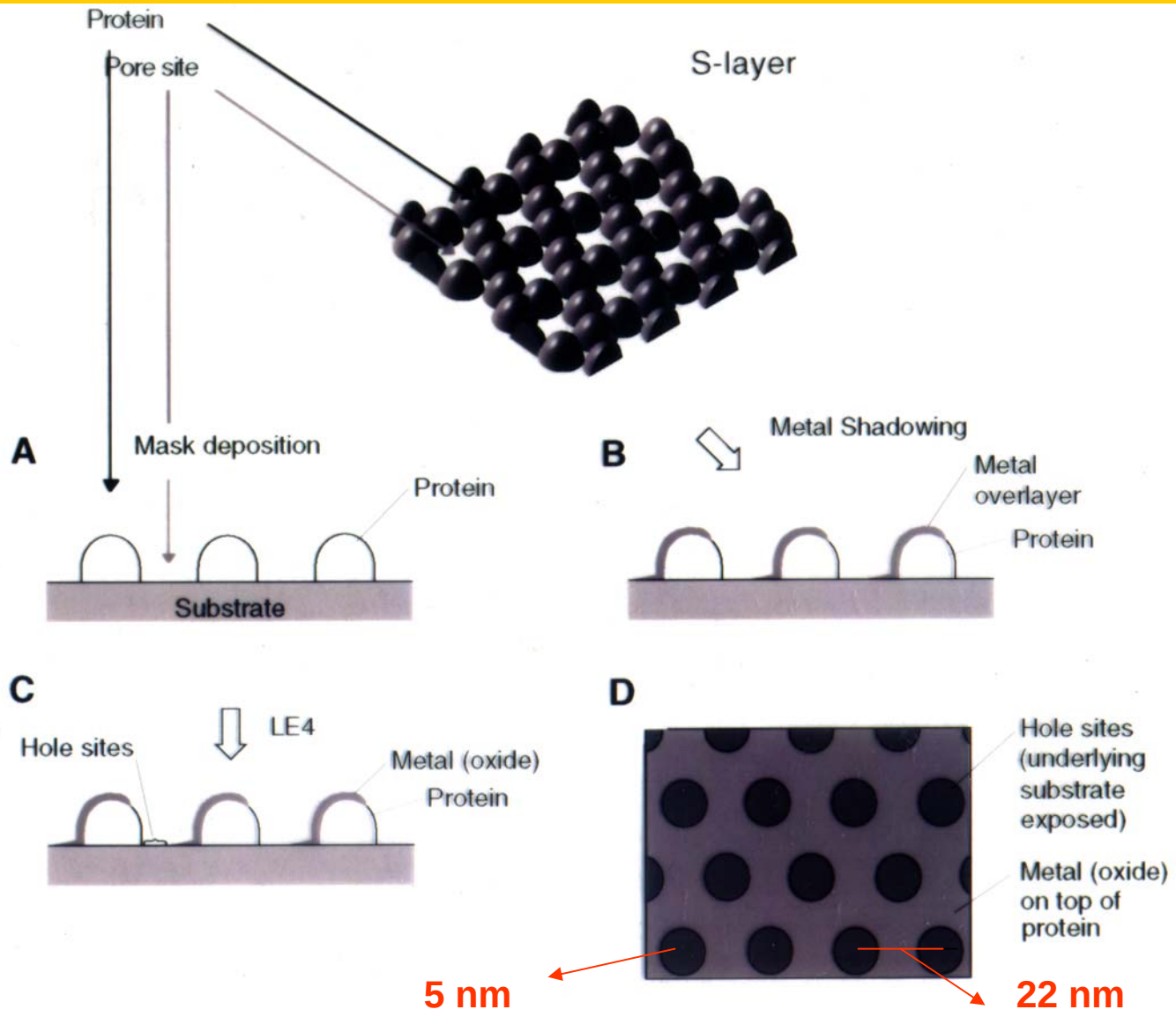
GaN/AlN/SiC Layered Structure



LE4 Rate: 300 nm / min vs.
ECR Rate: 100 nm/ min

LE4 is 3x Faster

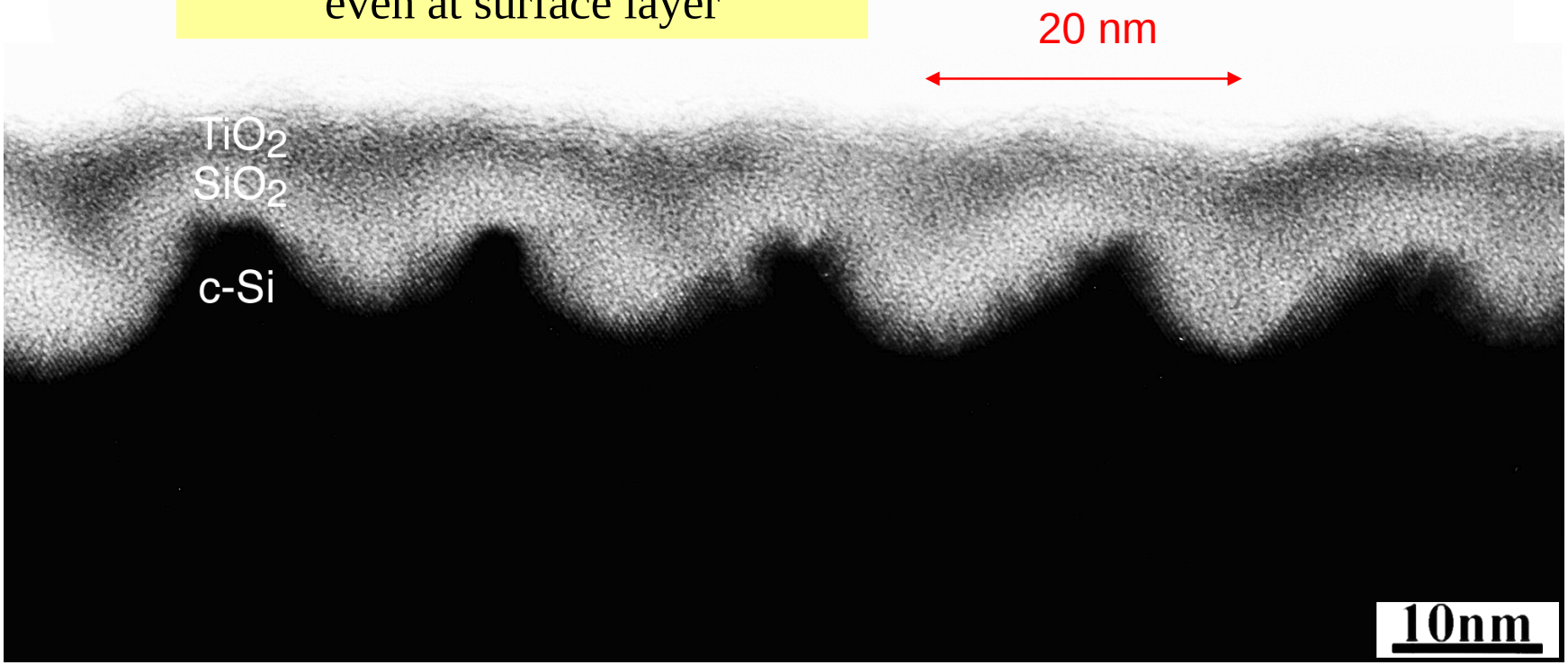
Formation of Biologically Derived Mask



Douglas, Devaud, and Clark, Science **257**, 642 (1992)

20-nm Si Structures via GRADINA

Lattice imaging shows no damage even at surface layer

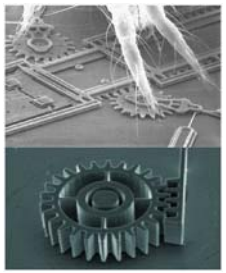


Basic etch science demonstrated for next 3 generations of Moore's Law

The rest is engineering: scale up GRADINA for 12-in wafers

Multiple Markets

> $5B (2004E)



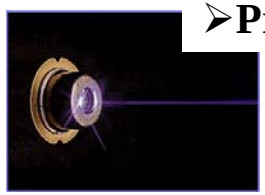
> Production model 2004

> $10B (2005E)

➢R&D model 2003;
➢Prodn. model 2004

> $5B (2002E)

➢R&D model 2002;
➢Prodn. model 2003



Laser Diode

Substrate Cleaning

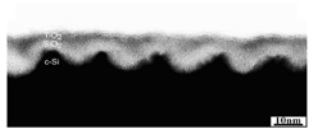
HB-LED

Systine Gradina Platform

MEMS

Power Amplifier

0.02 Micron Si

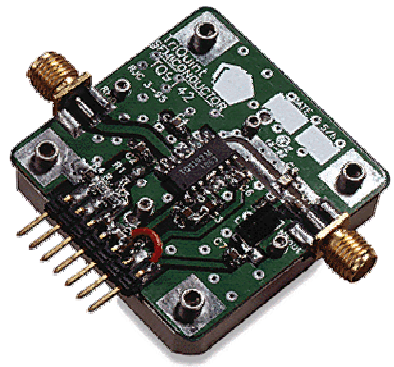


> $300B (2003E)

> $4B (2003E)

➢R&D model 2002;
➢Prodn. model 2003

> $20B (2003E)



➢R&D model 2002
➢Prodn. model 2003

> Production model 2005

Systine Inc.

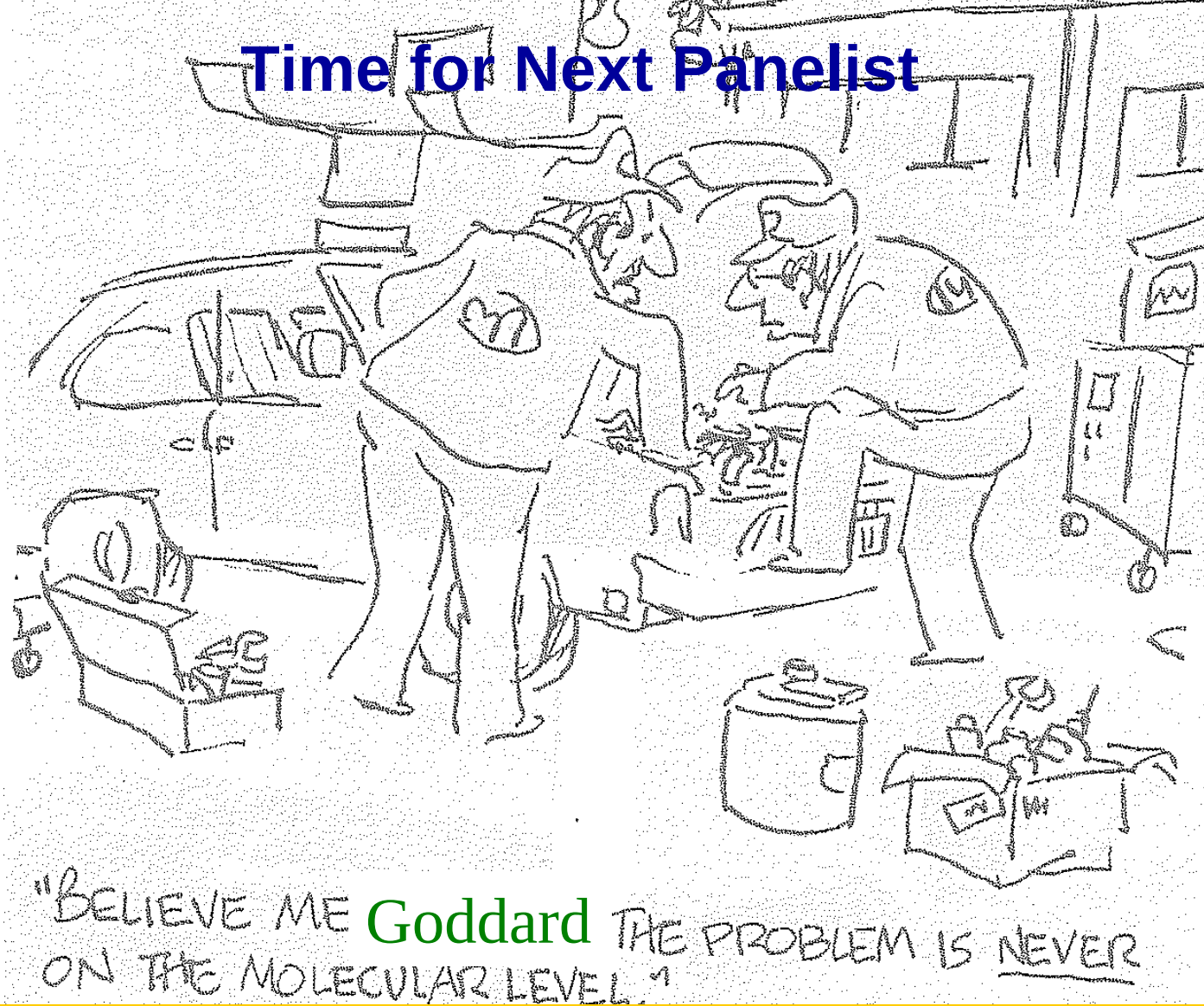
Incorporated (in Md) to commercialize the LEEE technology to produce the Gradina Advanced Electron Etching tool

Located in Pasadena CA.

Cofounders Pat Gillis (UCLA), Samir Janz (CalPoly), Bill Goddard (Caltech) plus 3 faculty at Georgia Tech, and North Carolina State Univ. Early support by SBIR grants plus founder funds.

Have developed and demonstrated prototypes for GaN, GaAs, InP, and Si.
Now seeking a Series A round to rapidly transition from protypes to production of research instruments needed to qualify Gradina for production

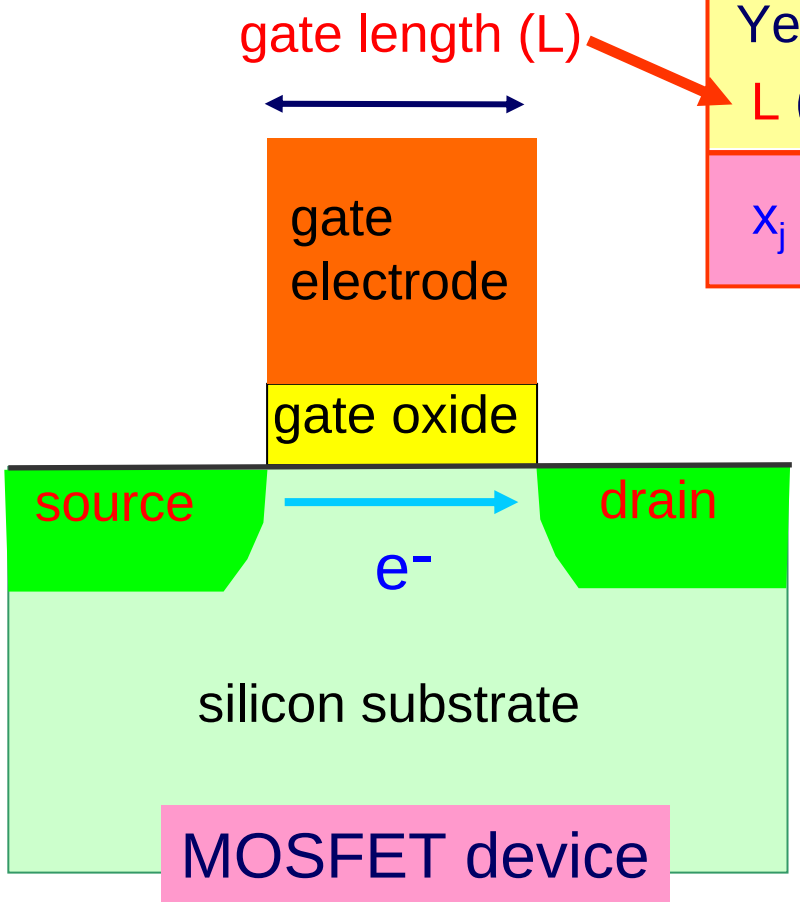
Support people:
ARO
ONR
NIH
NSF
DARPA
DOE ASCI
DOE FETL
ChevronTexaco
Seiko-Epson
General Motors
Asahi Kasei
Beckman Institute
Facilities (computers)
DARPA DURIP
NSF MRI
IBM SUR
Dell
Software
Schrodinger
Accelrys (MSI)



William Goddard PhD (Engr. Sci. 1965,Caltech) advisor: Pol Duwez
Pol Duwez DSc (1933, Brussels) advisor: Emile Henriot
Emile Henriot DSc (Phys, 1912, Sorbonne, Paris) advisor: Marie Curie
Marie Curie DSc (1903, Ecole Phys. Chim. Ind, Paris) advisor: Becquerel

GODDA

Illustration of using Multiscale modeling to explain a problem in Ultrashallow junction fabrication



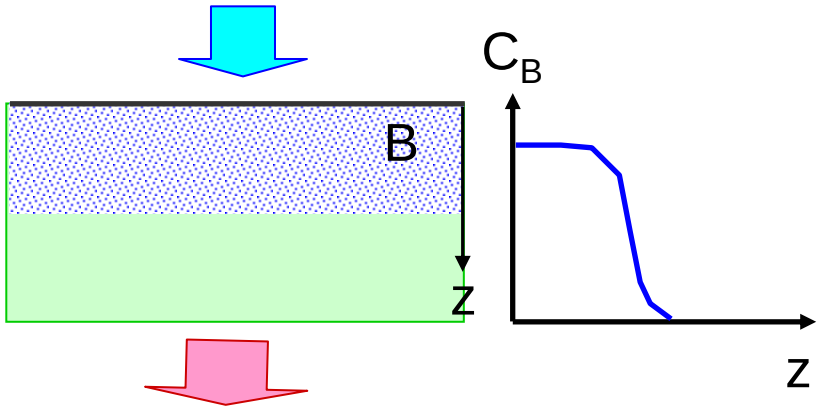
Year	2001	2004	2007	2010
L (μm)	(0.18)	(0.13)	(0.10)	(0.07)
x_j (nm)	30-80	20-70	15-45	10-30

Junction depth (x_j)

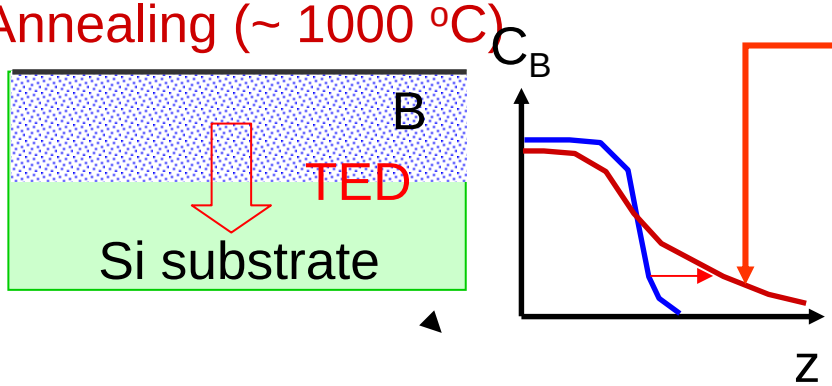
Greatly decreased gate length (100 nm) requires ultrashallow junctions (30nm) to minimize short channel effects.

What are the issues?

B^+ implantation (< 1 keV)



Annealing (~ 1000 °C)



Process requirements

- maximize dopant activation
- minimize dopant diffusion
- attain box-like doping profiles

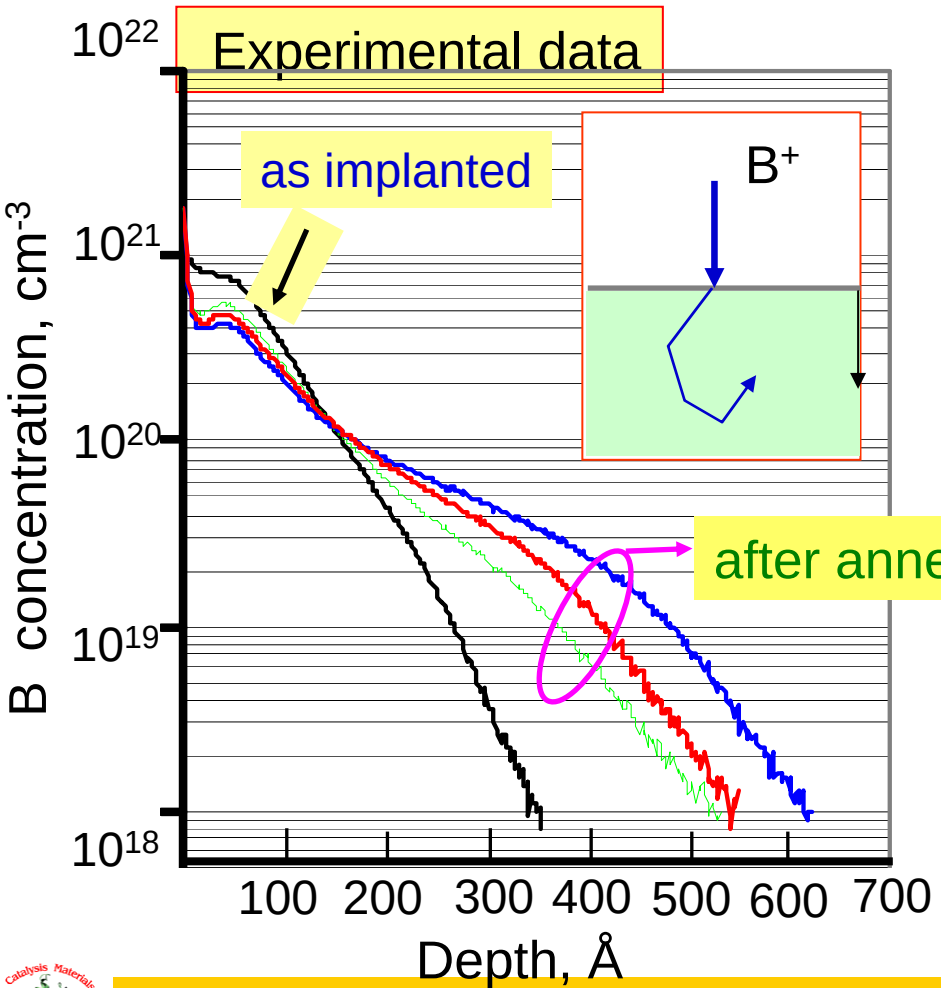
Requires Better understanding of

- low-energy implantation
- transient enhanced dopant diffusion (TED)
- defect/dopant clustering

*Requires Development of **predictive** numerical models*

Multiscale modeling and simulation

Technological Problem: Transient Enhanced Diffusion. Get long range tail.
Made worse by pronounced shoulder What causes it?
We found that it is due to a combination of Bs-SiI migration + BsB migration



explanation/
prediction

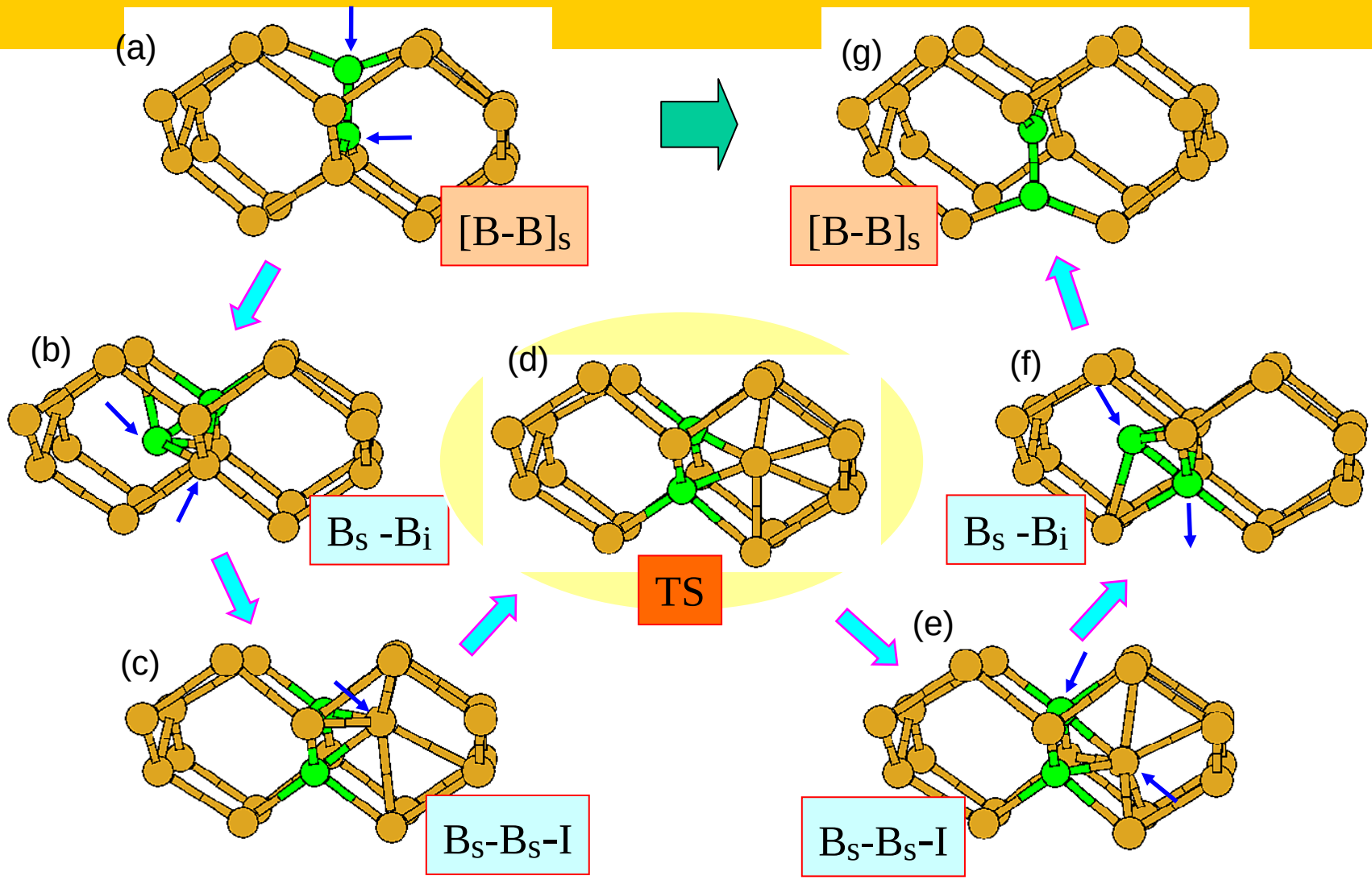
validation

Kinetic Monte Carlo simulations
[long time (>1 sec)]

fundamental data

Atomic-scale calculations
- density functional theory
- tight binding MD
- classical MD

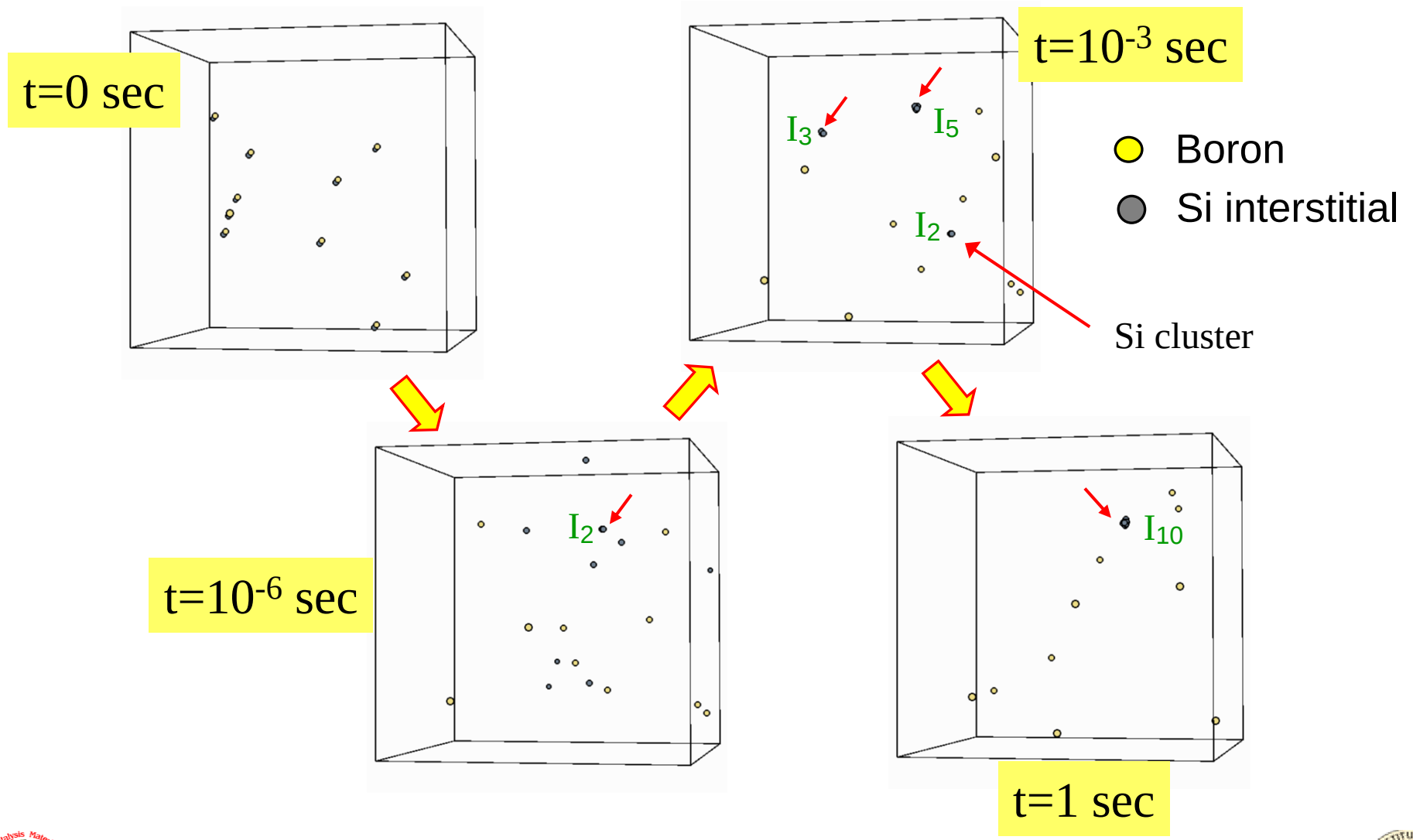
Critical discovery from QM: a pathway for diffusion of B dimers



Orange balls = Si atoms **green balls = B atoms**

diffusion pathway for a boron-boron pair.

Kinetic Monte Carlo simulation
(C_B=C_{si}=10^{19} cm^{-3}, T=900 K)



Diffusion profile evolution: experimental vs. simulation

Multiscale simulation provides quantitative agreement with experimental depth profiles. Thus can use theory to predict distributions for various configurations of the microdevice and various annealing protocols