

Nano-scale modeling with Undergraduates at Prairie View A&M University

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2006 Summer School on Computational Materials
Science: Ab Initio Molecular Dynamics Simulation
Methods in Chemistry



**Prairie View A&M
University**

Purpose

- Introduce the research and education environment at Prairie View A&M University, TX
 - Difference between research intense university and teaching intense university
- Current research activities in my group
 - Nanotube modeling
 - Protein modeling
 - Making a living machine

http://www.pvamu.edu


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 **PRAIRIE VIEW A&M UNIVERSITY**
A Member of the Texas A&M University System

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A Legacy of Greatness

During this year long celebration of 130 years, Prairie View A&M University honors its heritage and traditions, alumni, students, faculty and staff. While commemorating the past, future excellence must be the impetus.

What do the years mean? If they are filled with the honest sweat of service to humanity...the years are a benediction. Founded, symbolically, upon the ruins of a slave plantation, this college was authorized in the spirit of fair play...where wisdom would not allow vengeance to triumph over justice. The humble student, from every nook and cranny in the land, has left the echo of his laughter upon the wind, his hopes within the lurking shadows of our hills and by-ways. The giants, the world-shakers, have stood on our hill to mingle their search for truth with the fledgling's hope for life.

"The First Seventy-Five Years, 1876 - 1951, Prairie View A&M College of Texas" by Dr. George R. Woolfolk


Browse Categories **Colleges & Schools**

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PVAMU IN THE NEWS

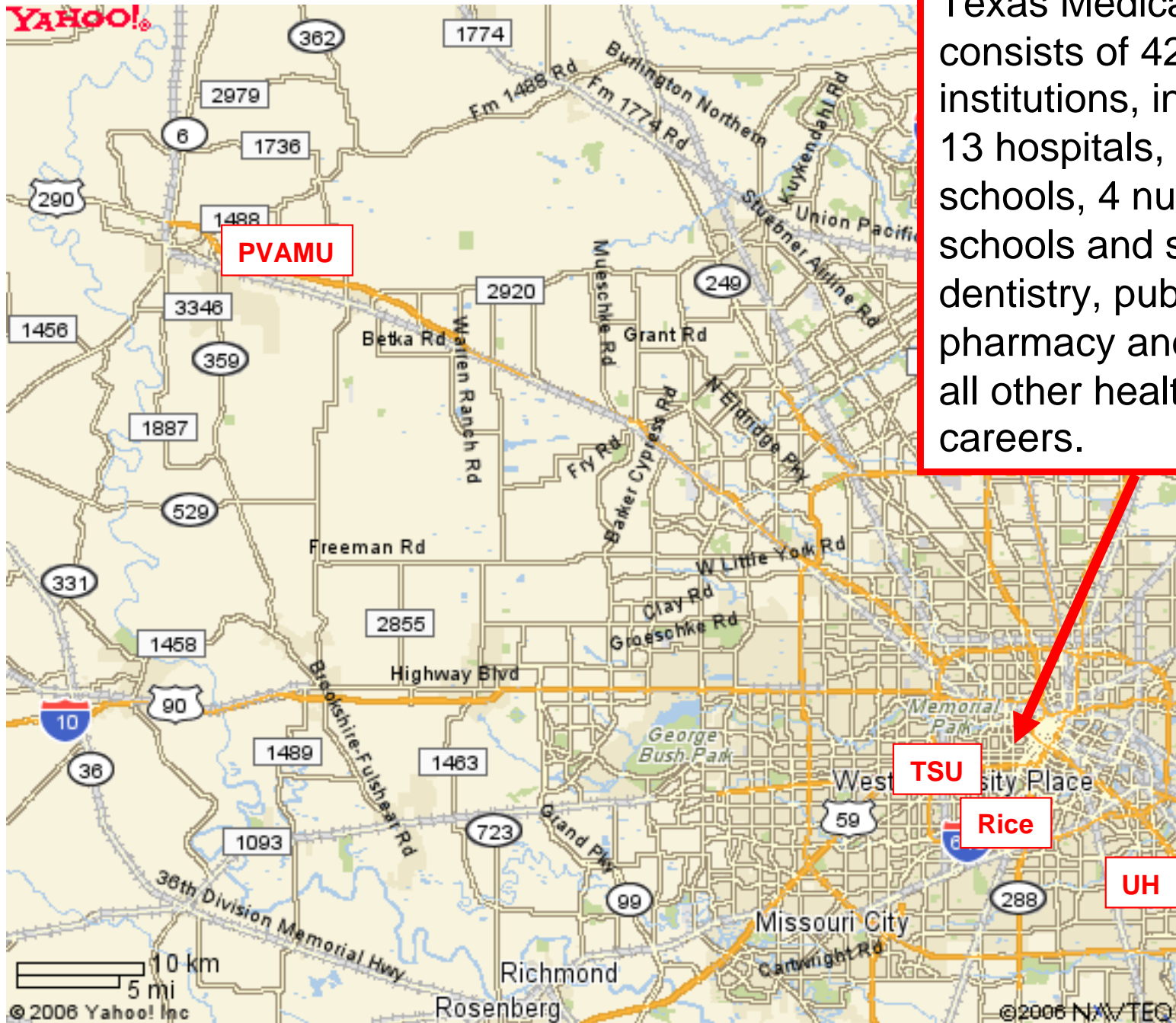
 **Tour de Pink Returns to Prairie View A&M For Another Cycle**
On **Sunday, September 10**, Prairie View A&M University will be the host site for the second annual Tour de Pink 2006 bicycle tour. [more](#)

 **Prairie View A&M University ACCESS Program Creates Hope For Returning New Orleans Students through Service Learning**

EXTEND THE VIEW
GIVING AT PVAMU

Summer Commencement
August 5, 2006
William "Billy" Nicks, Sr.
Health & Physical Education Building

http://www.pvamu.edu



Texas Medical Center consists of 42 institutions, including 13 hospitals, 2 medical schools, 4 nursing schools and schools of dentistry, public health, pharmacy and virtually all other health-related careers.

Prairie View A&M University

- Established in 1876 as Agriculture and Mechanical College for colored people
- PVAMU is a Historically Black University
- Part of the Texas A&M University System
- The second oldest institution of higher education in Texas
- A land grant institution (authorized under Morrill Acts of 1862 and 1890)

University Background

- PVAMU has nine colleges and schools.
- PVAMU currently offers
 - baccalaureate degrees in 39 academic majors
 - 31 master's degrees
 - four doctoral degree programs

PVAMU Mission

- Prairie View A&M University is dedicated to excellence in teaching, research and service. It is committed to achieving relevance in each component of its mission by addressing issues and proposing solutions through programs and services designed to **respond to the needs and aspirations** of individuals, families, organizations, agencies, schools, and communities--both rural and urban.
- The University's **public service programs** offered primarily through the Cooperative Extension Program target the State of Texas, both rural and urban counties. The University's research foci include extending knowledge in all disciplines offered and incorporating research-based experiences in both undergraduate and graduate students' academic development.

PVAMU Core Values

- Access and Quality
 - provide equal educational opportunity to increasing numbers of persons from unserved and underserved populations residing primarily among the economically and socially bypassed in the society
- Diversity
 - commitment to recruit, enroll, educate, and graduate students and to employ and advance faculty and staff without regard to age, ethnicity, gender, national origin, socioeconomic background, or educationally unrelated handicap
- Leadership
 - stimulate, initiate, and implement programs and services to both inspire and guide students, faculty, and staff in developing their self-confidence, self-discipline, and other requisites to becoming successful leaders in their professions and in their communities
- Relevance
 - respond to the need for highly literate, technologically competent graduates educated to excel in the 21st century work force
- Social Responsibility
 - promote active participation in constructive social change through volunteerism, leadership, and civic action on the part of its faculty, staff, and students

Research

- Like most small university, a push towards research involves undergraduate
- Encourage more students participation in faculty research activities as early as their sophomore year
- Improve research productivity and promote research
- Value of research experiences at the undergraduate level
 - Council on Undergraduate Research. Joint Statement of Principles in Support of Undergraduate Research, Scholarship, and Creative Activities. 2005



Prairie View State Normal and Industrial College, 1900

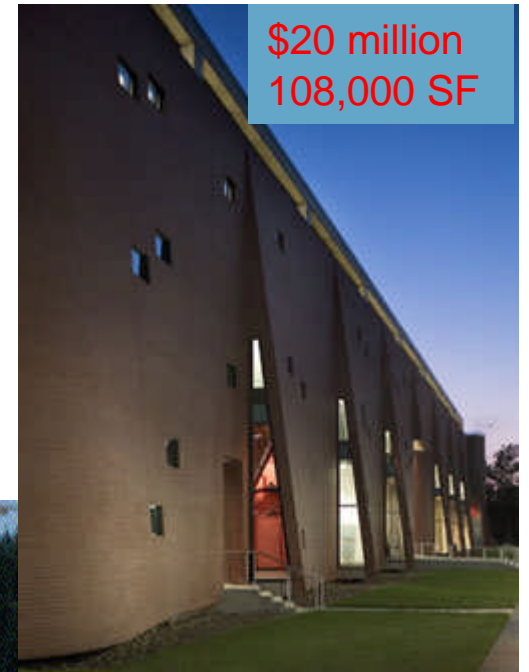
\$31 million
118,000 SF



\$23 million
157,322 SF



\$20 million
108,000 SF



\$12 million,
48,787 SF



Science Program at PVAMU

- The College of Arts and Sciences at PVAMU hosts all Science programs and courses.
- The New Science building hosts Biology, Chemistry, Physics Departments and Dean's Office



New Science Bldg

- The science building is a landmark for the university.
- All classrooms and offices are wired for technology.
- Distance learning lab has four flat-screen monitors for demonstrations and distance learning.
- The four-story building houses 17 biology labs, 15 chemistry labs, 9 physics labs, a 250-seat auditorium, seven lecture halls, various support functions and a greenhouse.



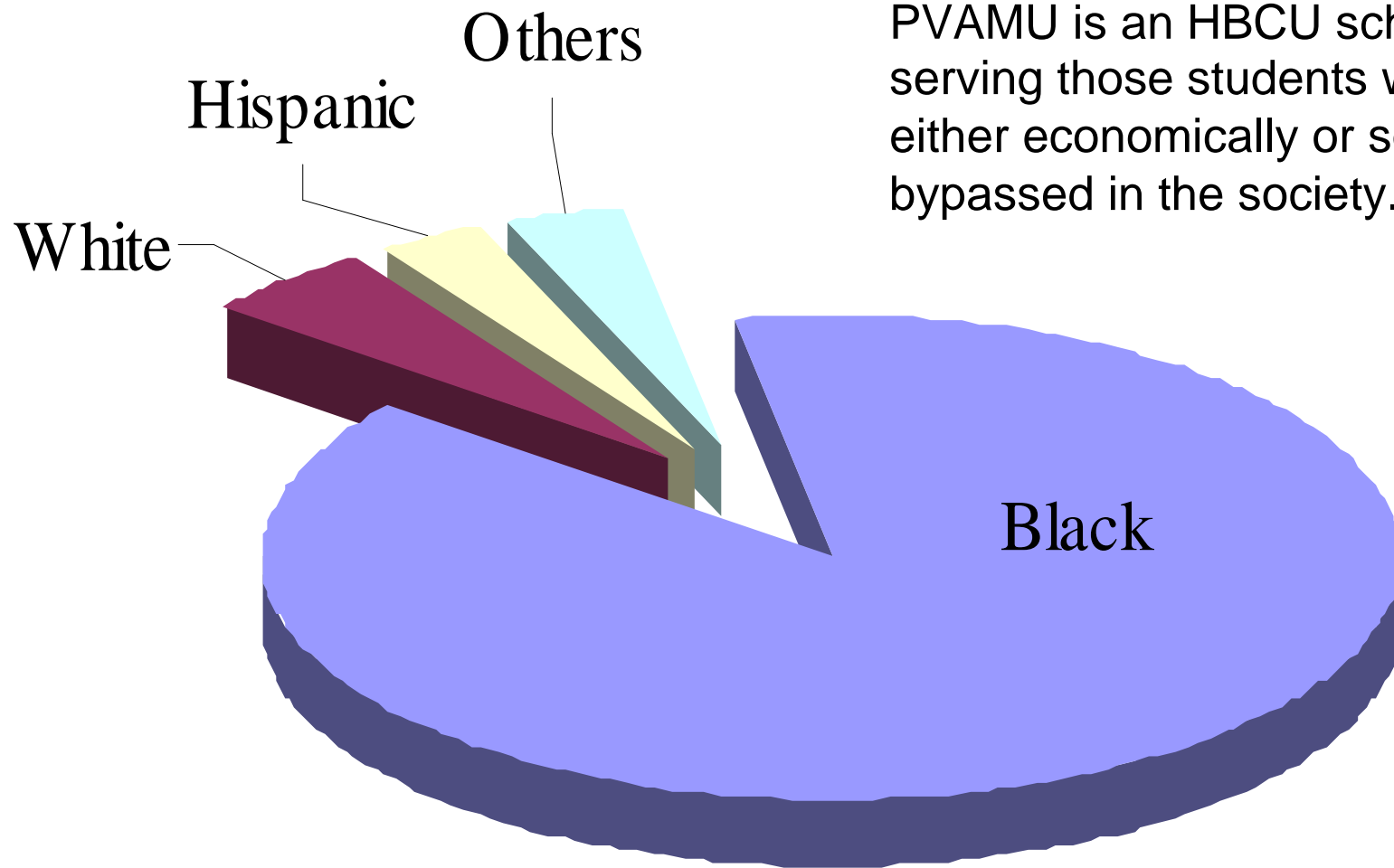
Major Research Equipments

- Major equipments to enhance research productivity in the Sciences
 - 400 MHz NMR in Chemistry,
 - DNA analyzer in Biology, and
 - SEM in Biology
 - Below 4K strong magnetic field
 -

Other facilities

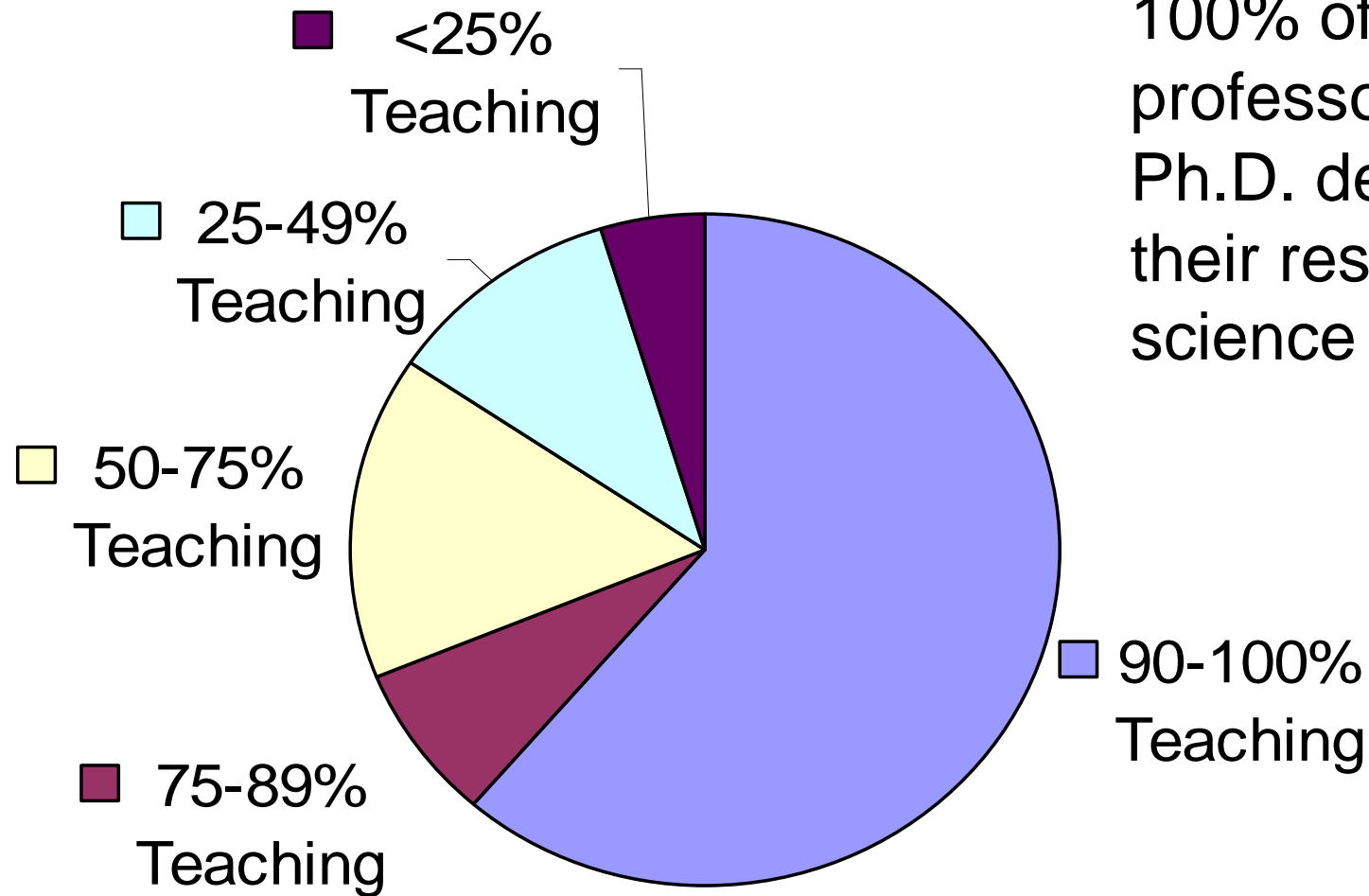
- Three newly renovated student dormitories; a new science building;
- Campus-wide wireless network;
- Dedicated 24-7 technology help desk;
- Distance learning center;
- Fifteen computer labs.

Current enrollment at PVAMU



PVAMU is an HBCU school serving those students who are either economically or socially bypassed in the society.

The current faculty teaching load



100% of these professors have Ph.D. degrees in their respective science disciplines.

Department of Chemistry

- 9 full-time faculty
- Inorganic (2), Computational Chemistry (1), Organic (2), Analytical (1), Physical (1) and BioChemistry (2)
- 400MHz NMR Lab,
- Instrumental Lab (AA, IR, UV-Vis, GCMS, HPLC, Magnetic Susceptibility)
- Analytical Lab (computerized interface)

Modeling Facility

A 16-node computing cluster at PV consisting of Dell 420 P-III computers. Each compute node has dual 733 MHz CPUs and 1 GB RAM.



Terminal PC in Computer labs can be used to access the two servers on PV campus and a Cornell supercomputer center.



Software available

- Material Studio
- NWChem
- ADF
- MOPAC2002
- Abintio
- VASP
- Spartan
- Dock
- AutoDock
- Maestro
(Schrödinger)
- CAChe
- Gaussian
- X-win 32

Research area one:

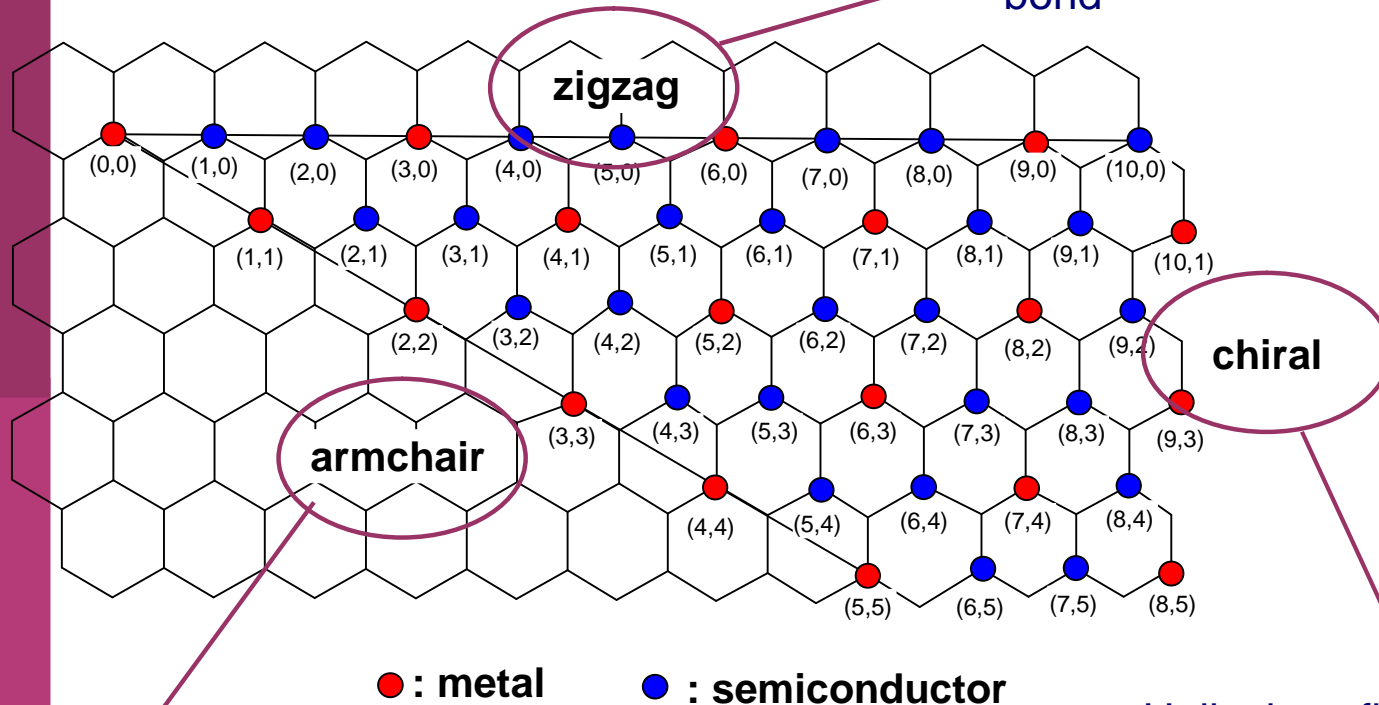
Carbon Nanotube for Shielding

- Conductivity and Shielding Effectiveness (SE) is used to evaluate the suitability of a shield. It is usually expressed by summing of losses of absorption, reflection and correction in terms of decibels.
- The electrically conductive polymer nanocomposite materials, as compared to conductive metal-based systems, offer substantial weight savings, flexibility, low-temperature processability, and tailored reproducible conductivity.

Carbon nanotubes: Rolled graphene layer

3 different ways of rolling:

Translational vector parallel to one C-C bond



Theoretical Tight Binding (TB) results have shown that ~ 1/3 are metallic and 2/3 are semiconducting

TB also predicts the band gap to be proportional to $1/d$, being d the SWNT diameter.

Helical configuration

Translational vector perpendicular to one C-C bond

These are known as the 1/3 and 1/d rules and were confirmed by experiments (Saito 2005)

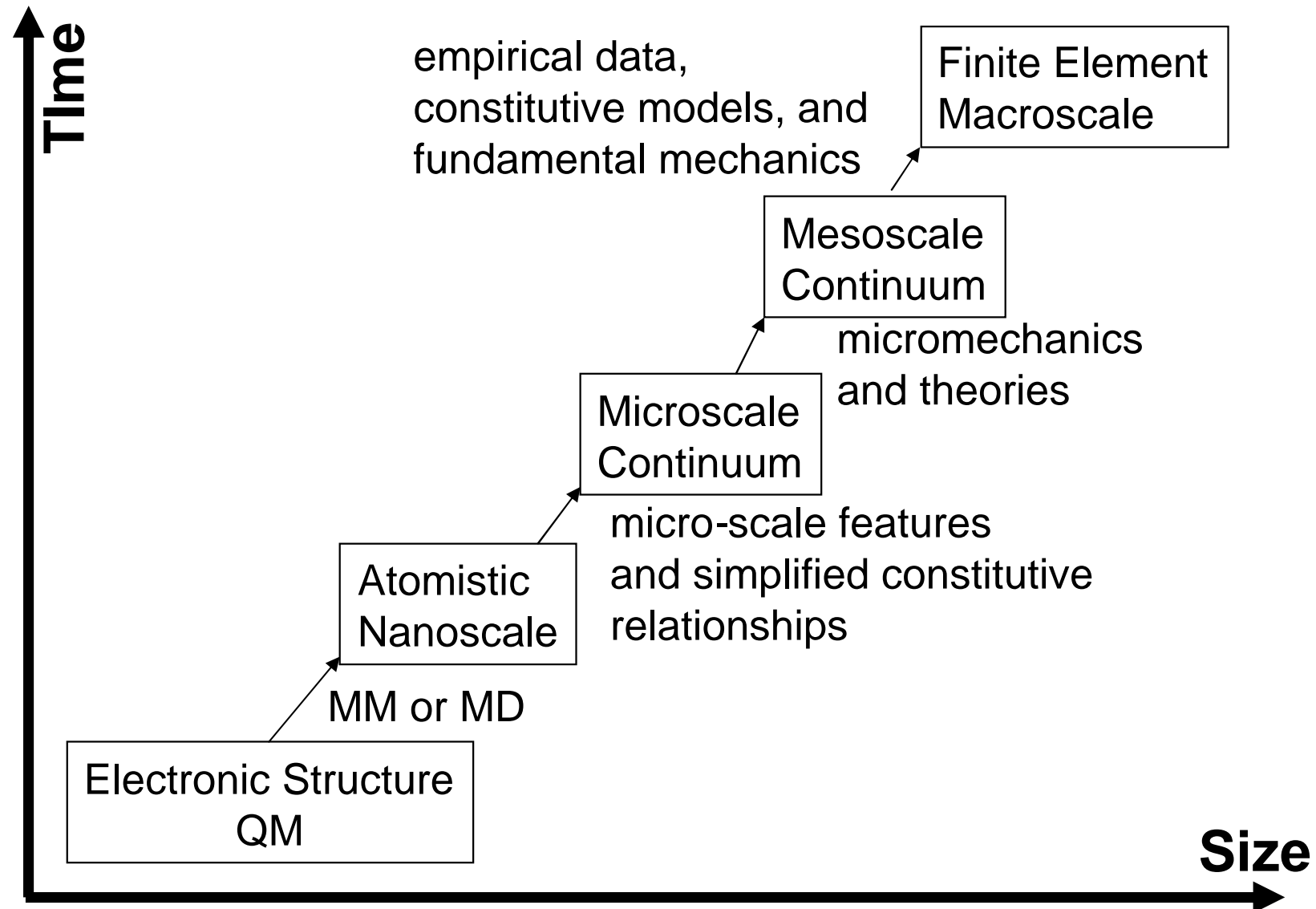
Theory and System

- Electronic properties of Carbon nanotube
 - Small energy gap (from a few meV for metallic to a few tenths of eV for semiconducting)
 - Depend on aromatic structure and wrap style
- Modeling of Carbon nanotube need
 - a large number of atoms
 - Sophisticated numerical tools
 - with multiple k point capability
- Powerful CPU + high fidelity model + 3D visualization

Theory and System

- Density Functional Theory provides a general framework for system with fewer than hundreds atoms
 - DFT-LDA with PW or GGA with HF
 - Vienna ab initio Simulation Package etc.
- Simulating the dynamic evolution as a function of time with up to 100,000 atoms
 - Need the electronic states and atomic forces from DFT modeling (Coupled first order differential eq.)
 - Meshless Local Petrov Galerkin method
 - MOPAC2002 etc.

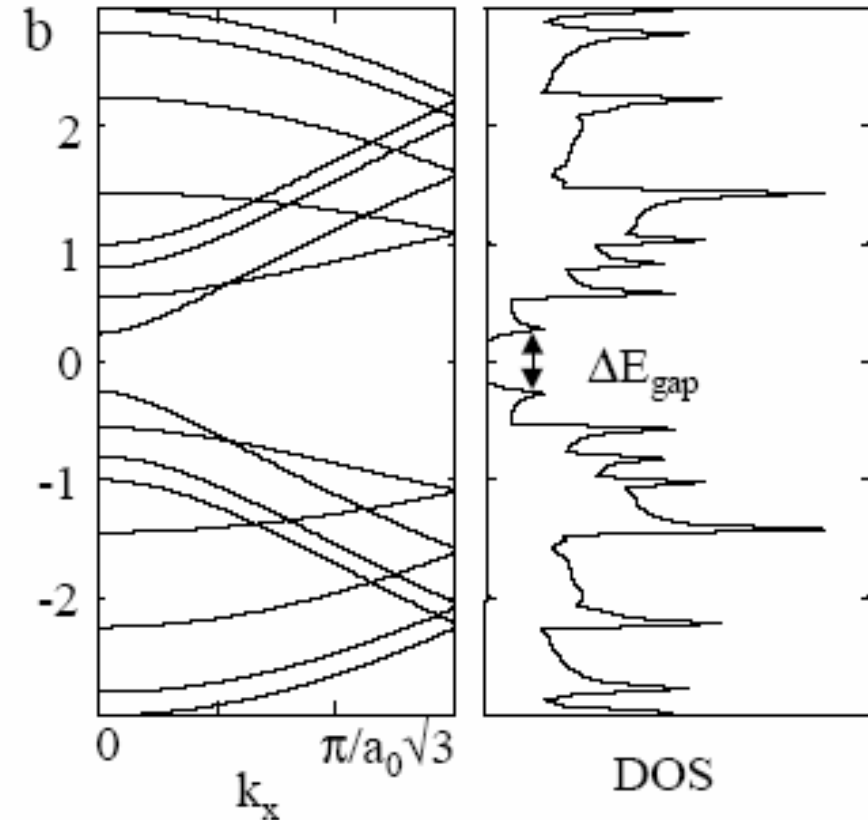
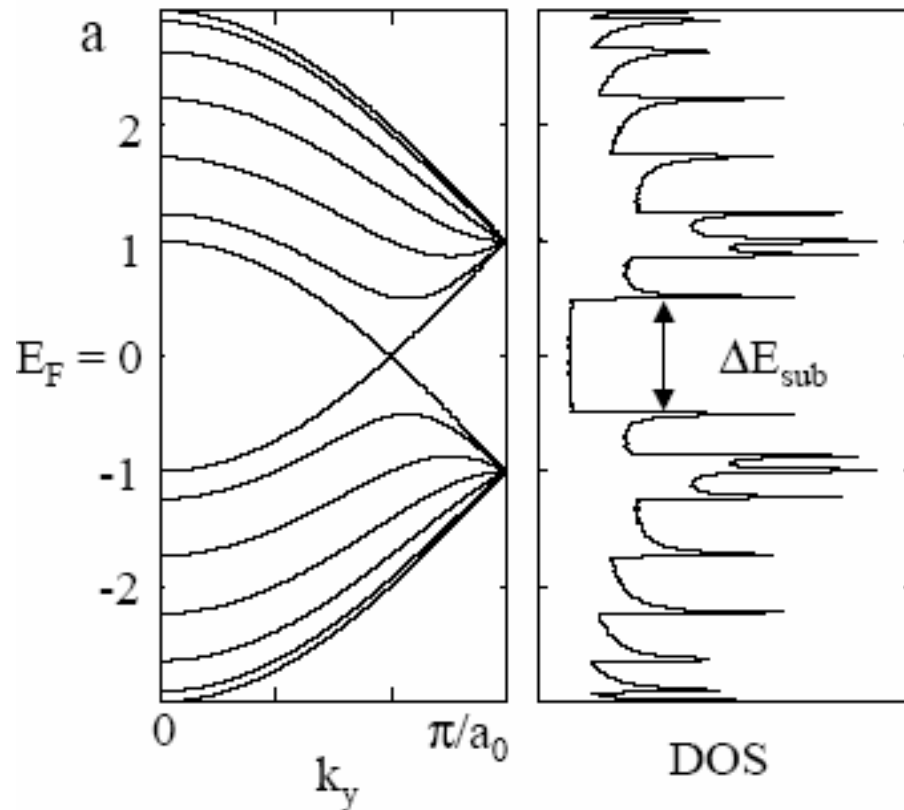
Modeling Approach



Electronic Structure

Metallic

Semiconducting

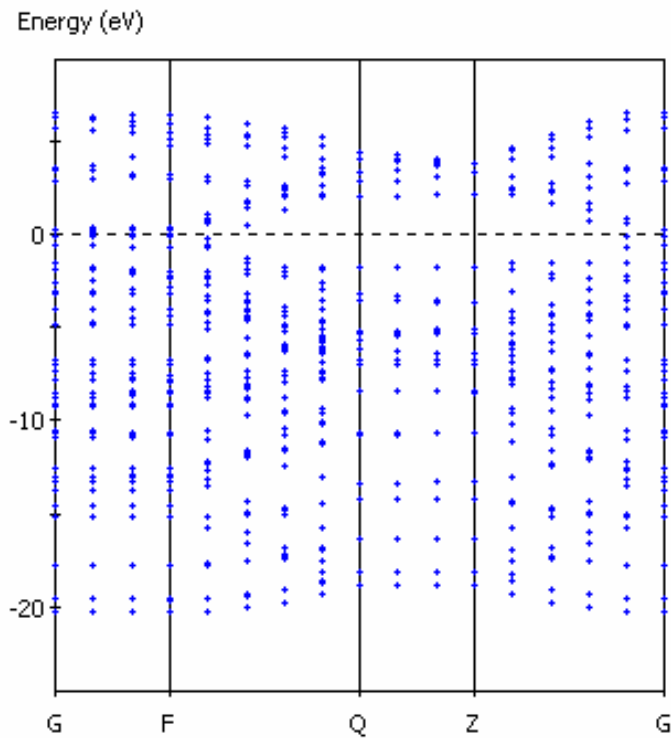


- * non-zero and constant DOS at E_F
- * Wide plateau

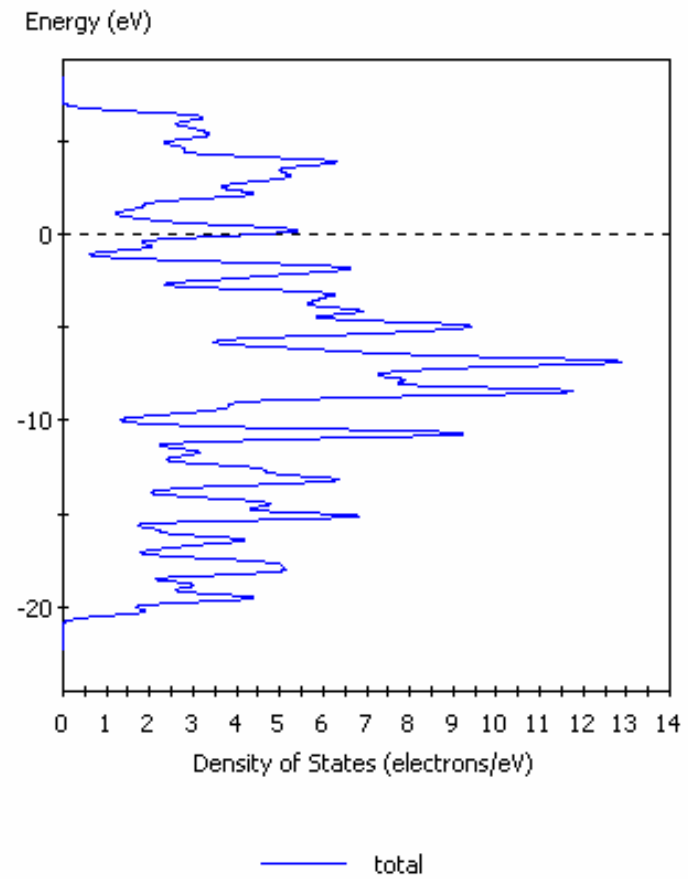
- * zero DOS at E_F
- * Small band gaps

6,0

CASTEP Band Structure

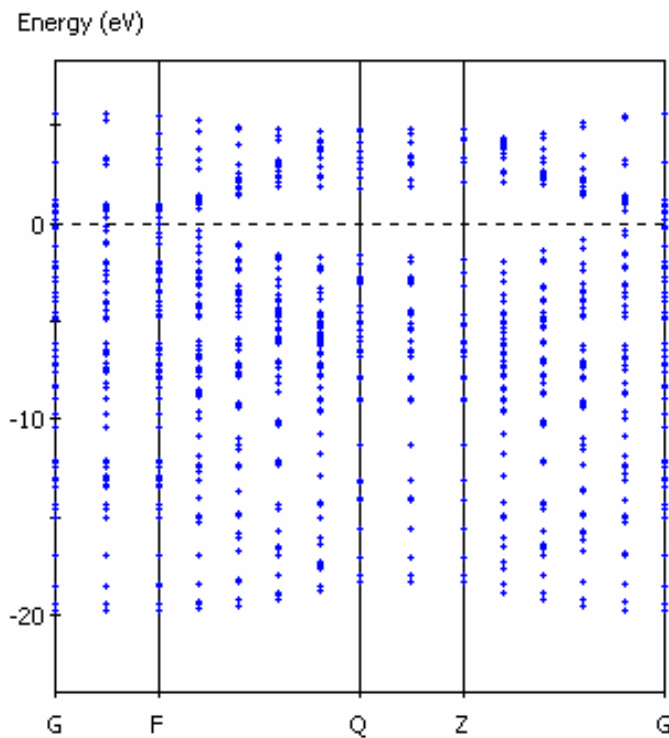


CASTEP Density of States

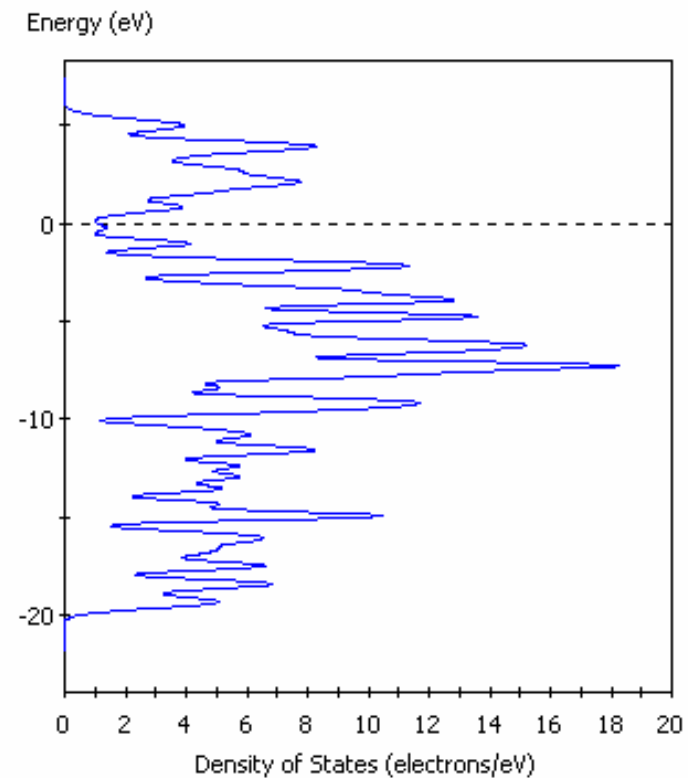


8,0 w/o opt

CASTEP Band Structure



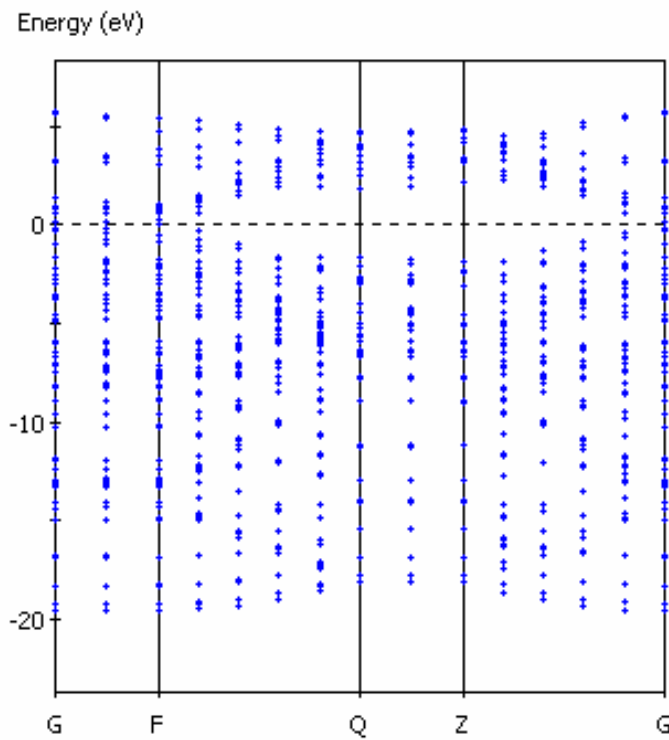
CASTEP Density of States



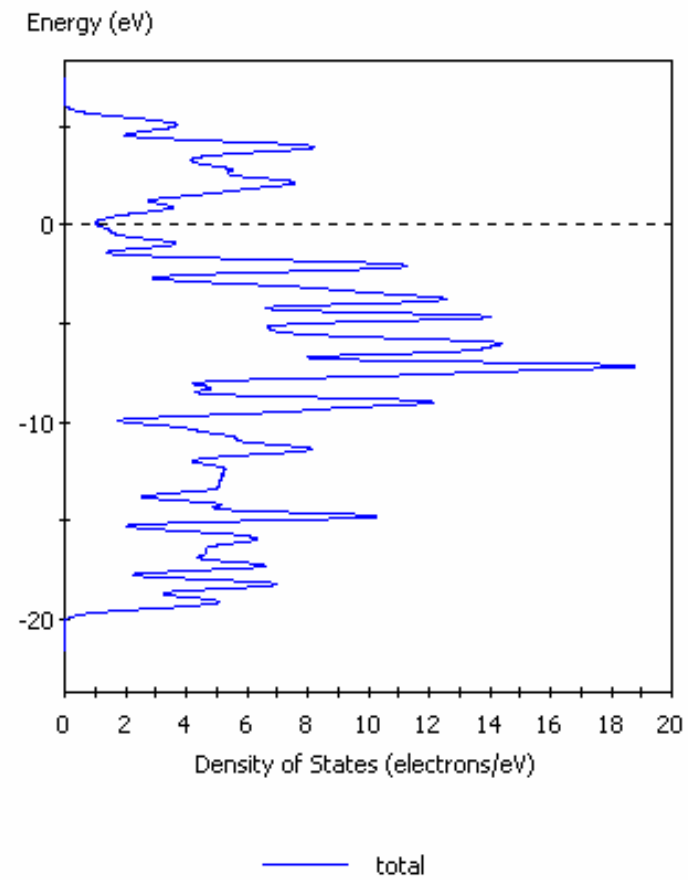
— total

8, 0

CASTEP Band Structure

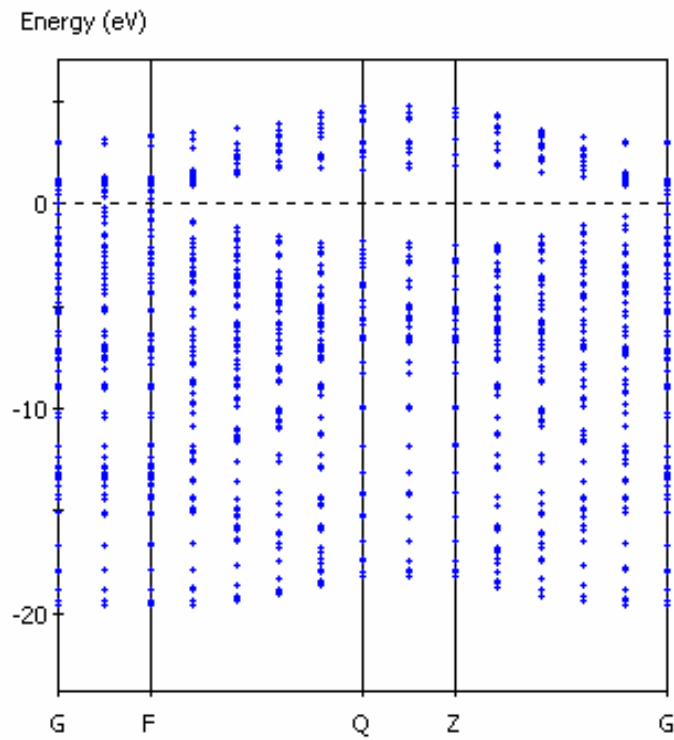


CASTEP Density of States

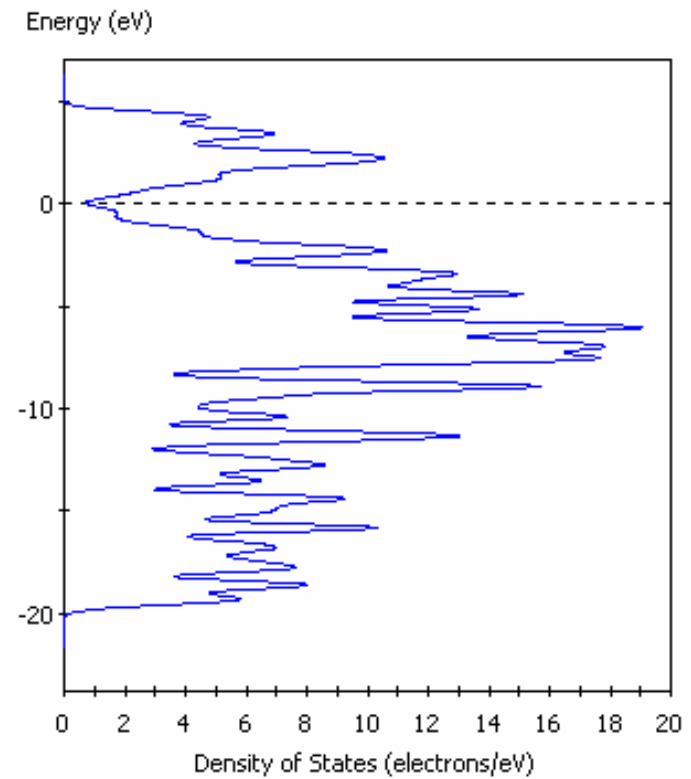


10, 0

CASTEP Band Structure

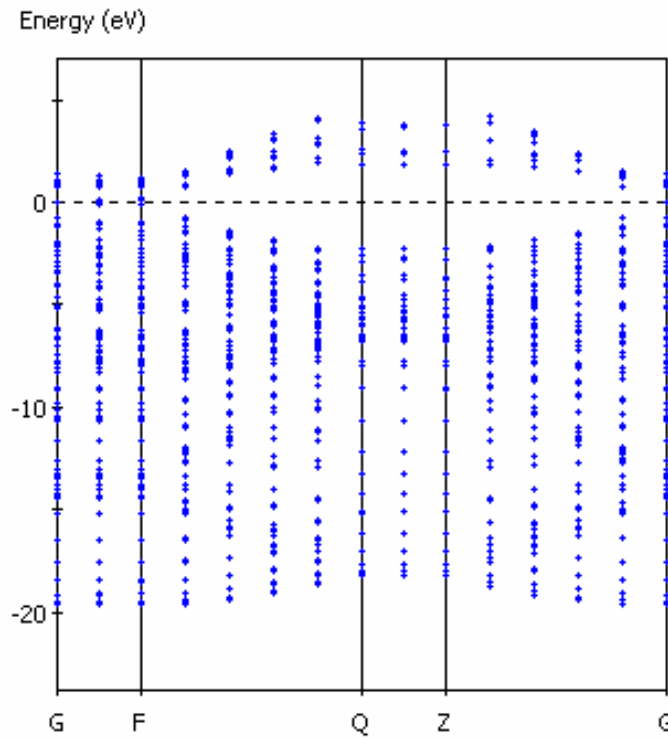


CASTEP Density of States

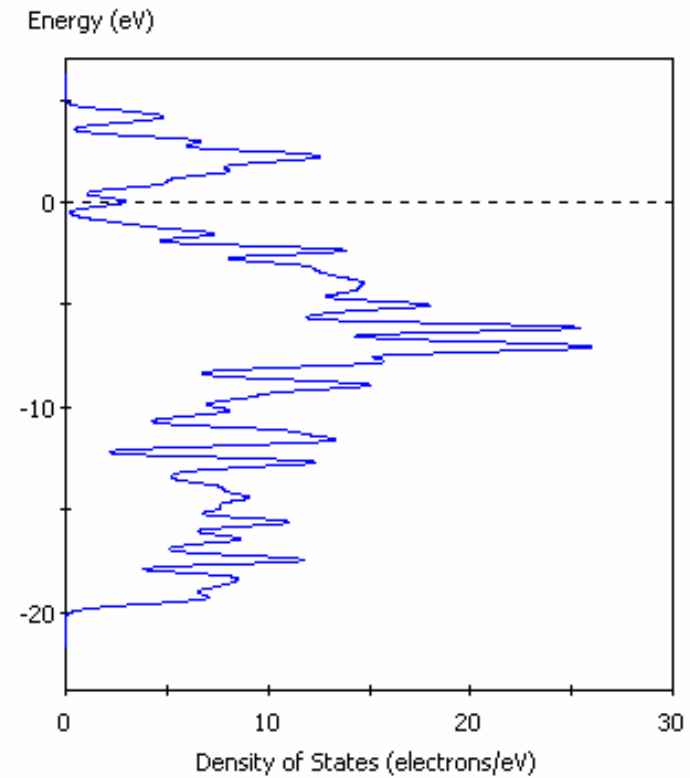


12, 0

CASTEP Band Structure

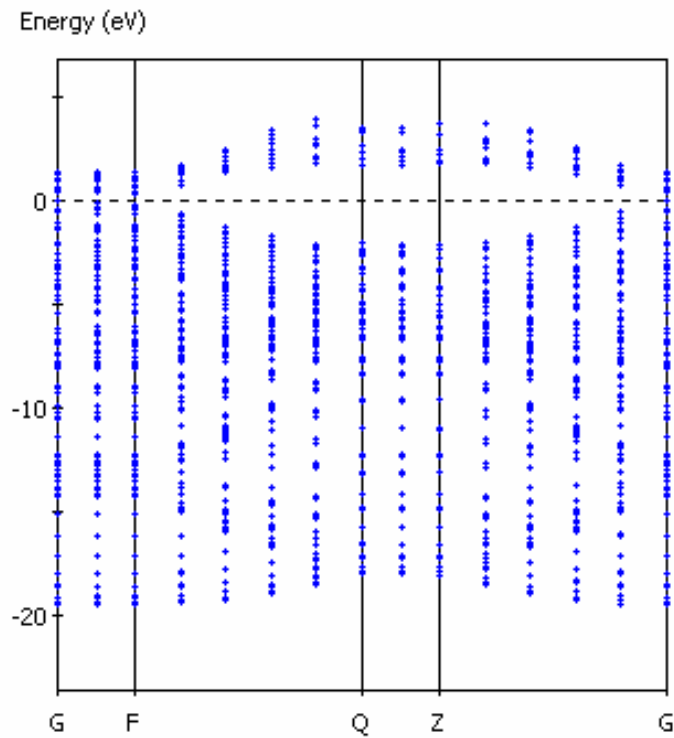


CASTEP Density of States

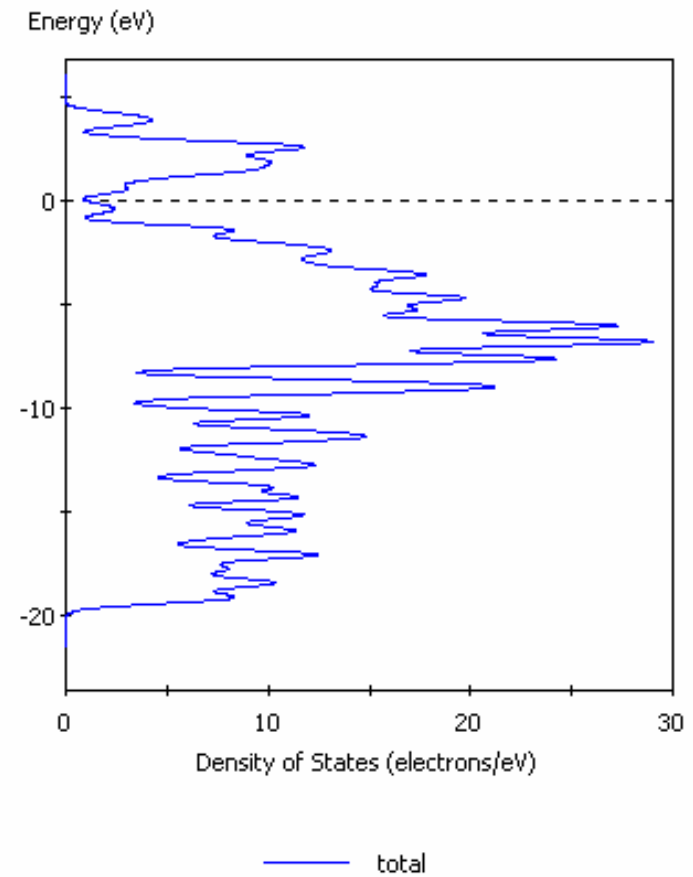


14, 0

CASTEP Band Structure



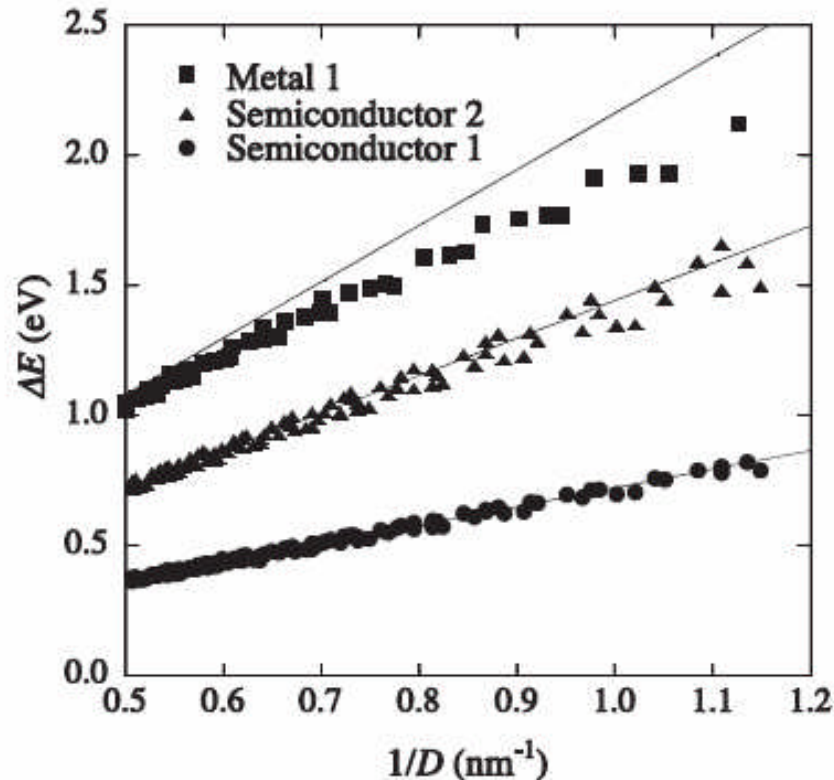
CASTEP Density of States



Some known results

- Software
 - CRYSTAL98 code
 - Material Studio
- DFT (LDA) or PBE (PW91)
 - More in house code
- Basis set

More known results



- LDA Energy separation of DOS peaks
- Semiconductor 1: separations of DOS peaks for the first valence-band peak to the first conduction-band peak
 - Semiconductor 2: the second peak-to-peak of semi-conducting tubes
 - Metal 1: the first peak-to-peak of metallic tubes

Saito 2005

Electronic Structure/DOS: Helical and rotational symmetries
methods to reduce carbon atoms into two; read-space grid to
solve LDA Kohn-Sham equation
Total E/Geom: plane wave basis method

More Problems than solutions

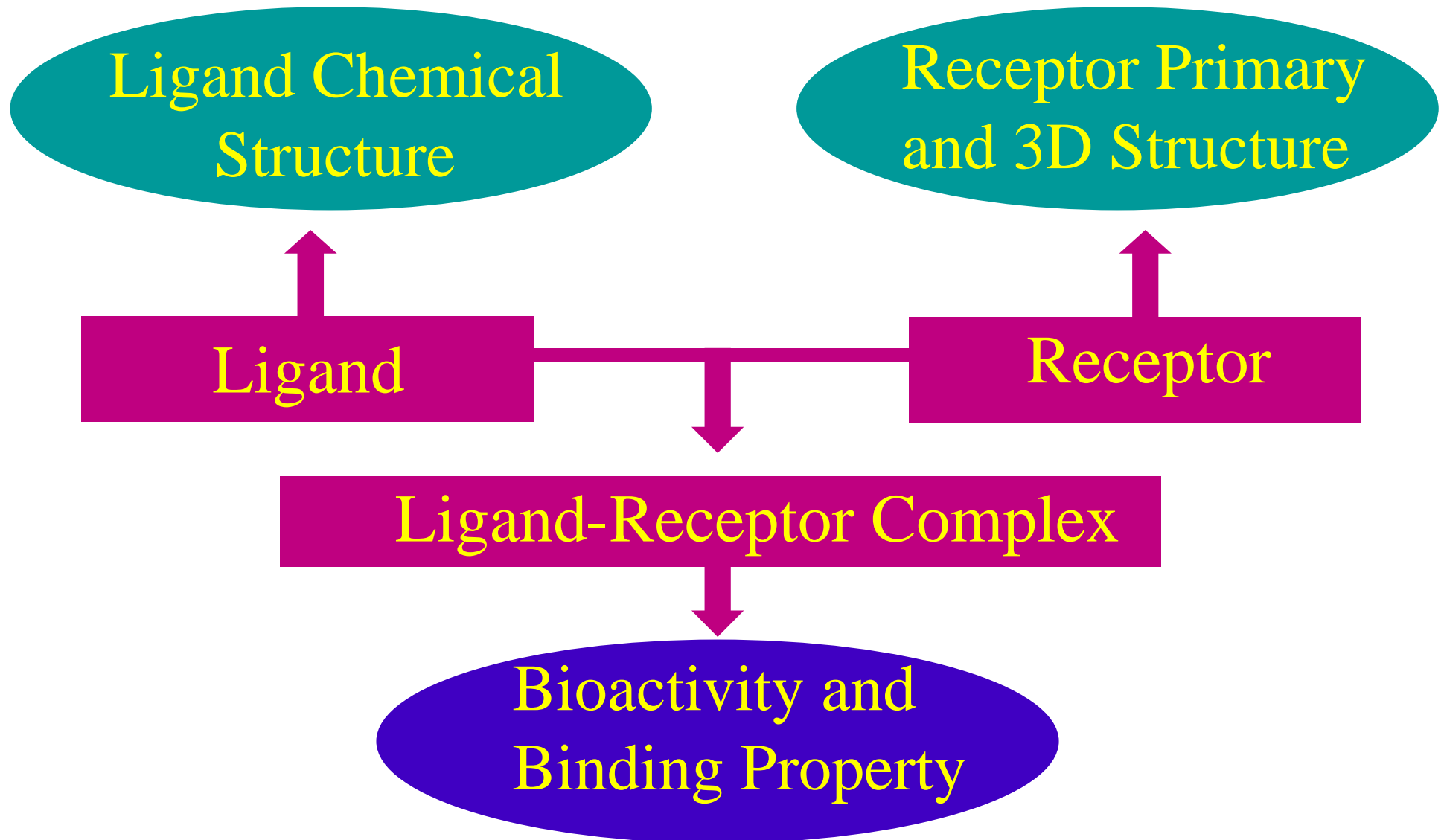
- How Brillouin Zone is sampled
 - Seven Monkhorst-Pack k-points along the Γ -X direction in the reciprocal space
- How electronic structure correlated to transport properties
 - Energy gap at Fermi level (qualitative)
- How the conductivity measured/modeled?
 - Tomonaga–Luttinger-liquid (TLL)
 - tunneling between the Fermi liquid (FL) and the TLL

Research area two:

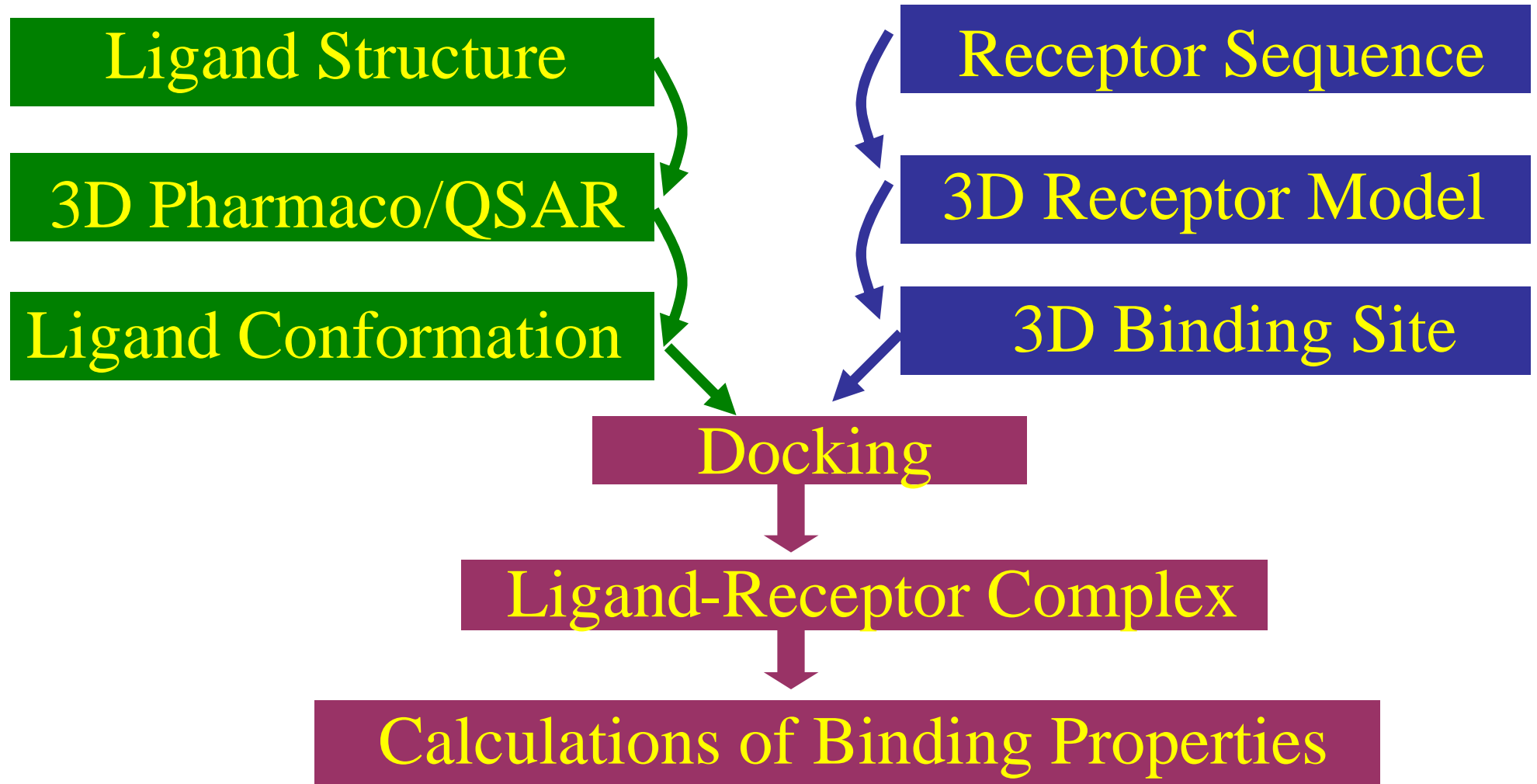
Protein Modeling

- Evaluate and assess the potential health and environmental effects of existing chemicals in our habitat
- Modeling and predicting the interaction between a small molecule and a biological macromolecule, such as receptor-ligand, enzyme-substrate, DNA-genotoxicant.
- Provide guidance for screening chemical toxicity based on the molecular target-toxicant paradigm is feasible with development of hardware and software.

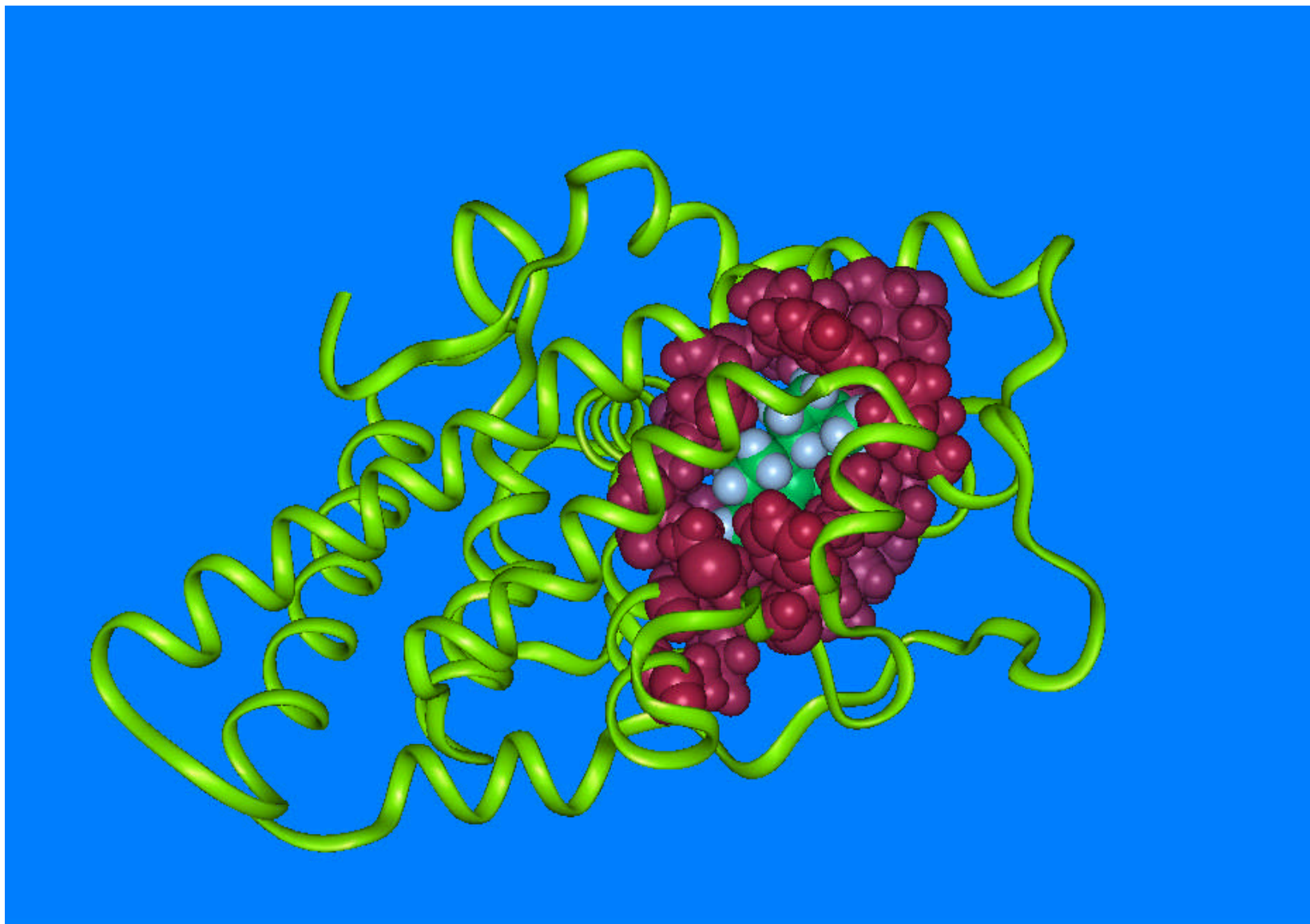
Ligand-Receptor Interaction



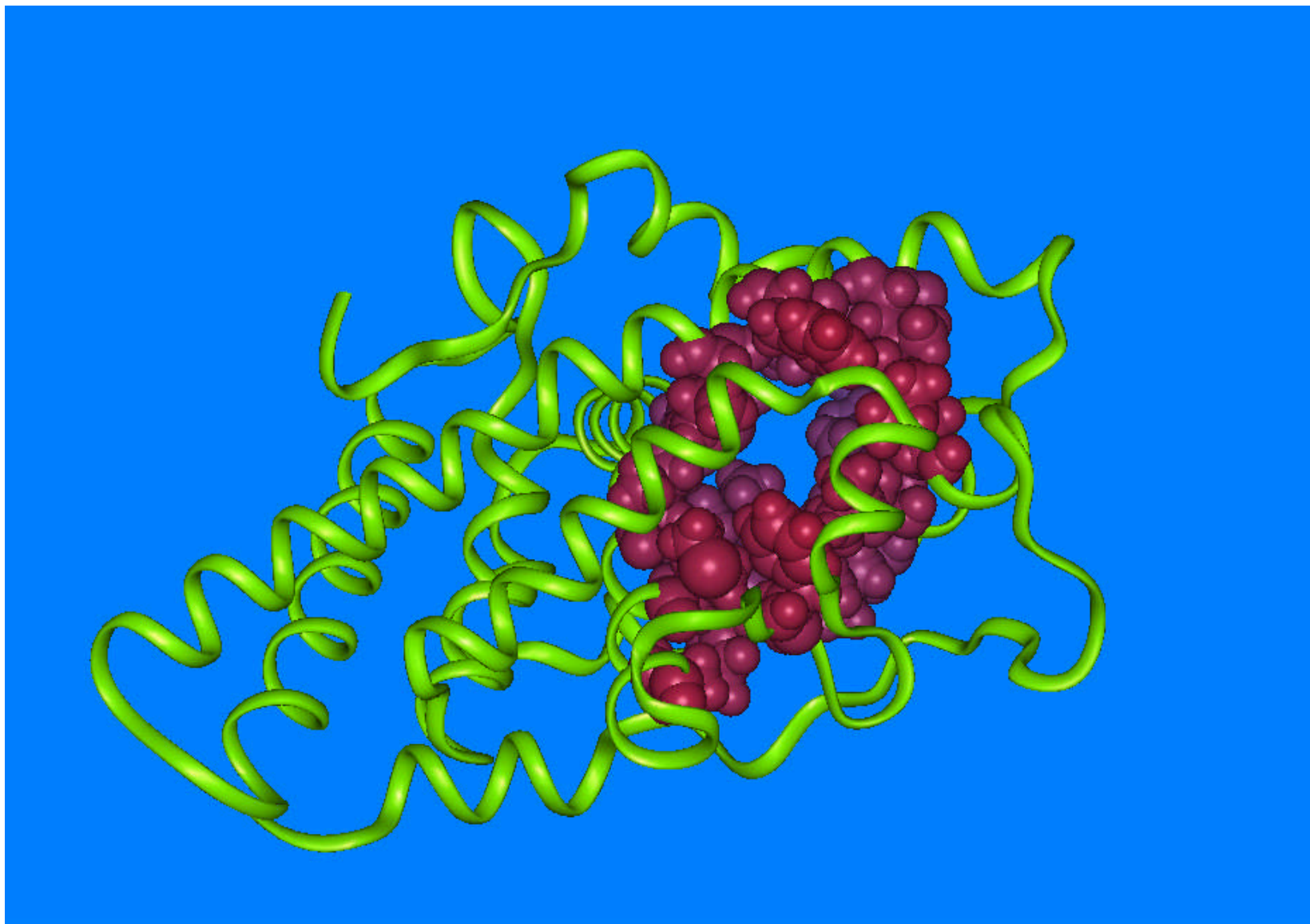
Modeling Ligand-Receptor Interaction



Work flow



Work flow



Work flow

The ligand is removed computationally to create a molecular target site for interested chemicals to be fitted (docked) into.

A library of potential target molecules are fitted (docked) into the molecular target site to find the best fit using Affinity, Glide, Dock, and AutoDock softwares.

Interaction energies, binding affinities etc are calculated

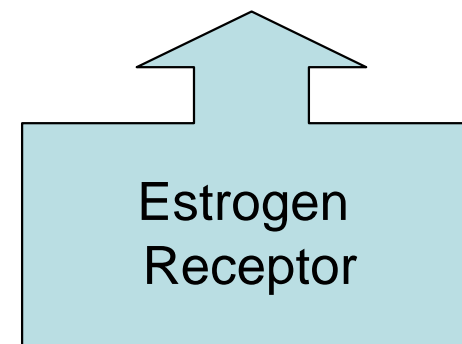
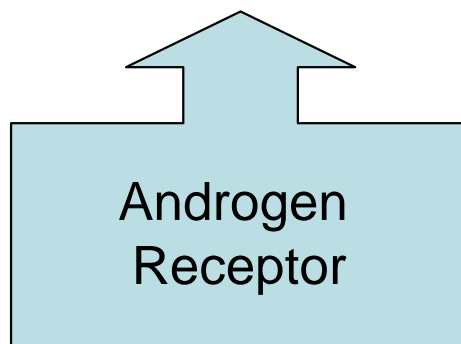
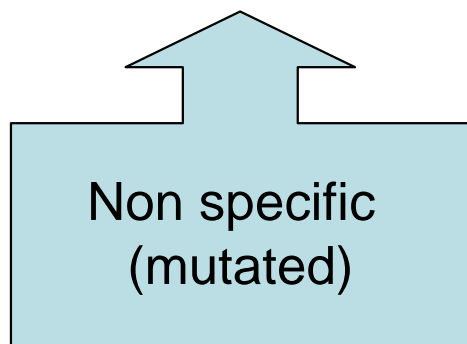
Results

	1GS4
Mibolerone	-10.27
Dihydrotestosterone	-9.97
TRENBOLONE	-9.79
R 1881	-10.12
5-ANDROSTAN-17-OL	-9.23
Testosterone	-9.98
6-Methyl-17-acetoxyprogesterone	-9.29
17b-Estradiol (E2)	-9.49
CYPROTERONE ACETATE	-7.94
4-androstenedione	-9.30
PROMEGESTONE	-10.10
Progesterone	-10.38
Corticosterone	-9.99
LINURON	-7.11
Bisphenol A	-7.89
Vinclozolin	-7.04
Estriol	-9.89
Aldosterone	-10.47
PREGNENOLONE	-10.61

(####: means no docking score)

Re-organize the docking results

The best interaction for each chemical		
1GS4 6-Methyl-17-acetoxyprogesterone CYPROTERONE ACETATE PROMEGESTONE Progesterone Corticosterone Aldosterone PREGNENOLONE	1I37 & 1I38 Mibolerone Dihydrotestosterone TRENBOLONE R 1881 5-ANDROSTAN-17-OL Testosterone 4-androstenedione LINURON Vinclozolin	1GWR & 1GWQ 17b-Estradiol (E2) Bisphenol A Estriol



Factors that control outcome

- Quality of the acceptor and ligand (charges, protonation state, solvation)
- Available functional groups on ligand
- Shape of the ligand
- Flexibility of acceptor and ligand (rotomer)
- Conformational space search
- Trainable scoring function (software)

Research area three: Making a living machine

- (old idea) Genetic engineering=“asking” *E. coli* to make a single protein from another organism.
- (new idea) A bacterium is a “chassis or building block” and used as a circuit board
- The only HBCU in the International Genetically Engineered Machine competition

Purpose

- To design and construct a new biological system and redesign the natural ones
- BioBricks DNA parts are engineered and standardized
- These BioBricks are free to participated institutes and used like lego style
- Big question: play god?

More information

- International Genetically Engineered Machine (iGEM)
 - [Parts.mit.edu/wiki/index.php/Main_Page](http://parts.mit.edu/wiki/index.php/Main_Page)



Thank you!

<http://www.pvamu.edu>