A Scientific and Engineering Computing Cluster Focusing on the Modeling and Simulation of Materials

Where is UNT?

UNIVERSITY OF NORTH TEXAS
CASCaM
CENTER FOR ADVANCED SCIENTIFIC COMPUTING AND MODELING

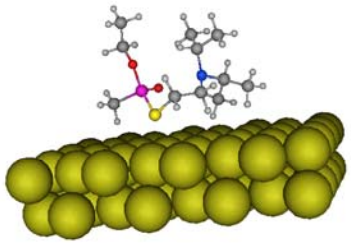
- college town
- close to DFW metroplex
- 4th largest TX university: >35,000 students

UNT Chemistry

- Largest chem dept in region
- 23 full-time faculty
- ≈ 100 grad students and post-doctorals

Cundari Group participates in ***CASCaM***, one of the largest and most diverse comp chem groups in the US!

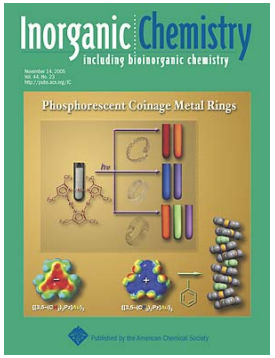
New Chemistry Building



UNIVERSITY OF NORTH TEXAS

CASCaM

CENTER FOR ADVANCED SCIENTIFIC COMPUTING AND MODELING

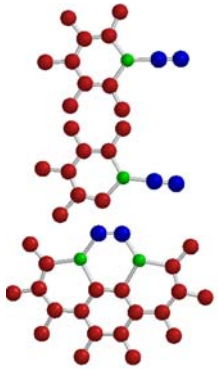


Core Competencies

- Materials Modeling
- Interfacing with Experiment

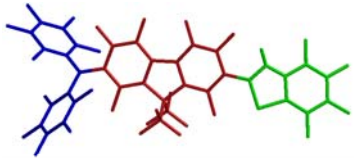
CASCaM At A Glance

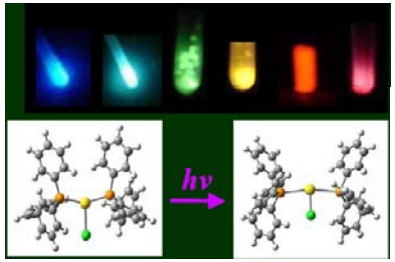
- 13 faculty
- cover all time and length scales
- ~50 researchers

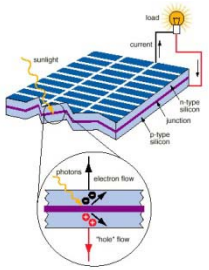


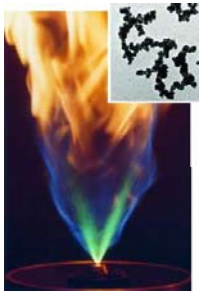
Currently Funded Projects

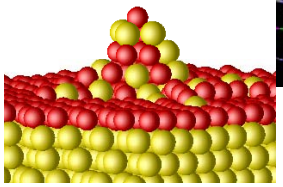
- Catalysis
- Photonics
- Flexible electronics
- Combustion chemistry
- Material fatigue

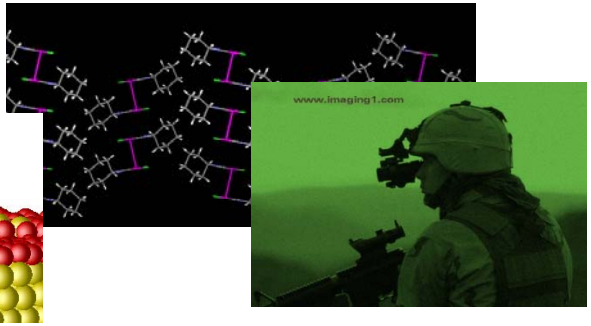




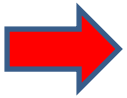


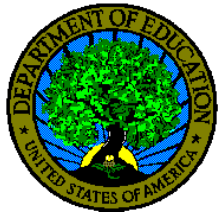




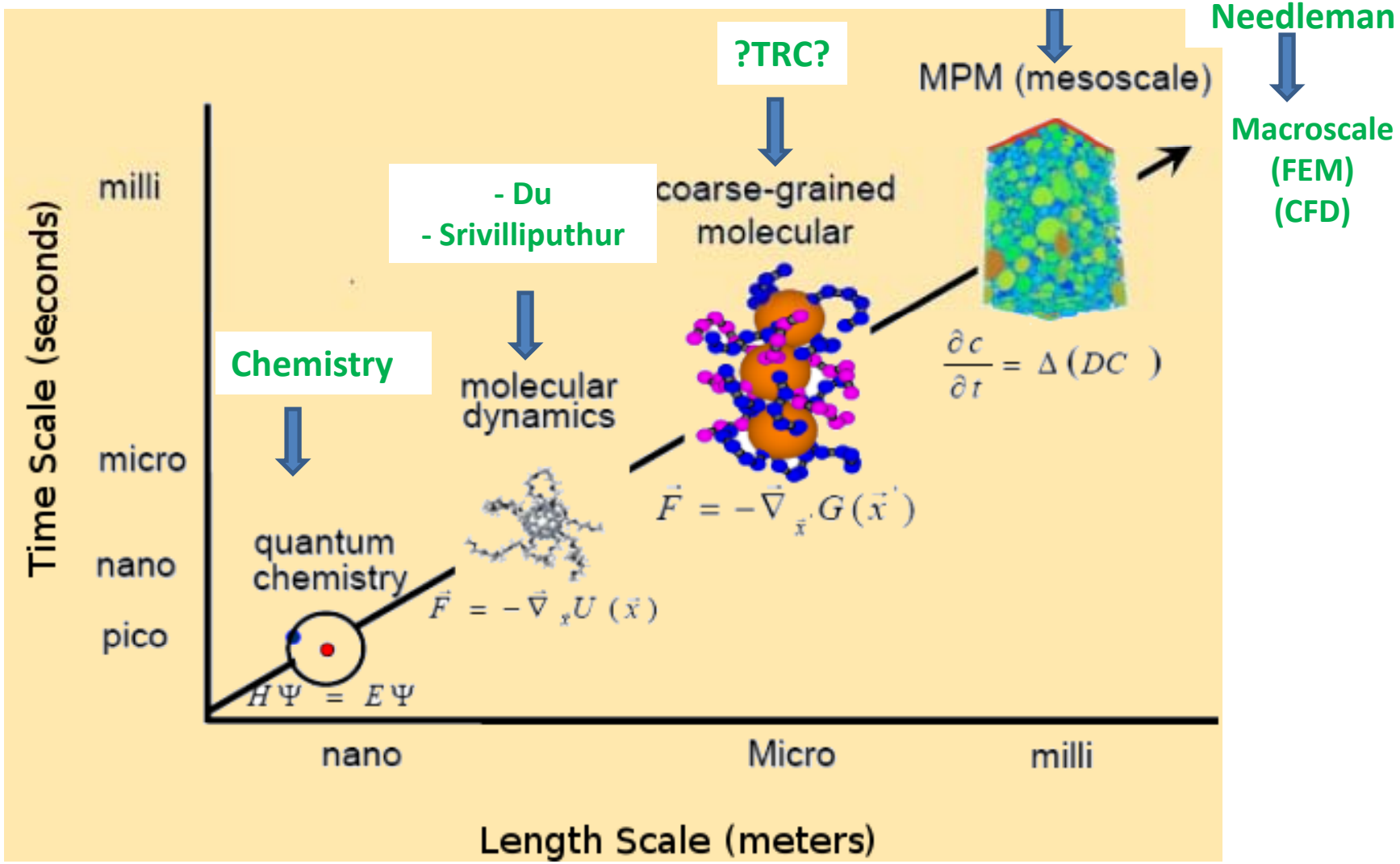


Current Sponsors





Expertise Across Time & Length Scales



Targets hires to “fill” and “bridge” the gaps in current expertise domains

Goals of the Modeling Cluster

1. **Extend** and consolidate current areas of strength
2. **Nurture** recent areas of modeling emphasis
3. **Diversify** UNT's expertise in modeling
4. **Integrate** UNT's modeling excellence with both on- and off-campus experimentalists

Make UNT a recognized leader in cross-disciplinary materials modeling research

Cross-Disciplinary Expertise

- **Chemistry**
  - Bagus
  - Borden
  - Cundari
  - Marshall
  - Wilson
  - Schwartz

- **Engineering**
  - Boetcher (M&EE)
  - Du (MS&E)
  - Feng (M&EE)
  - Needleman (MS&E)
  - Srivilliputhur (MS&E)

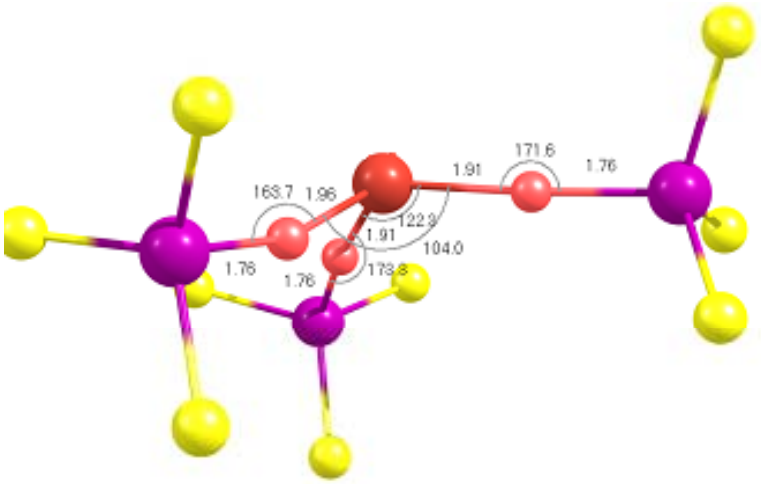
UNIVERSITY OF NORTH TEXAS
CASCaM
CENTER FOR ADVANCED SCIENTIFIC COMPUTING AND MODELING

MS&E: Materials Science and Engineering
M&EE: Mechanical and Energy Engineering

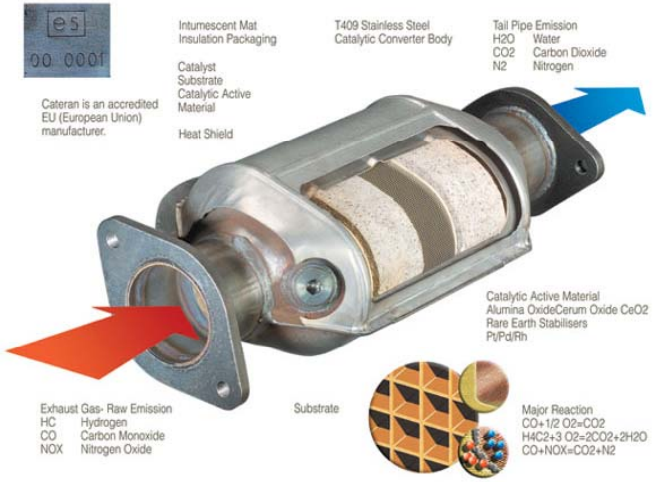
Dr. Thomas R. Cundari, Co-Director, **CASCaM**

Regents Professor of Chemistry
Editor, Reviews in Computational Chemistry
Editorial Board, Journal of Computational Information and Modeling

Catalysis, Energy Related Research, Project ISES,Biomodeling



Model catalyst for destruction of the pollutant NOx.



www.cateran.com.au/cateran/images/technical.jpg

Better catalysts are needed for more efficient destruction of NO_x in automotive catalytic converters.

Current Funding Sponsors

NSF

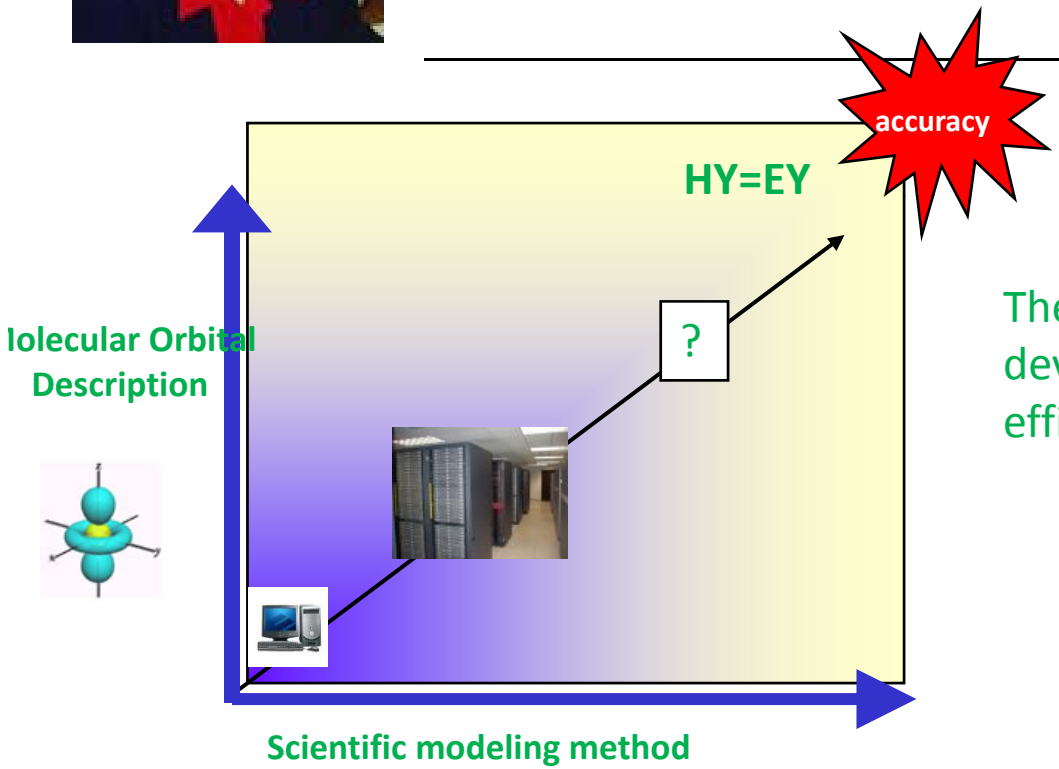
DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

AIR FORCE RESEARCH LABORATORY

Texas Higher Education Coordinating Board

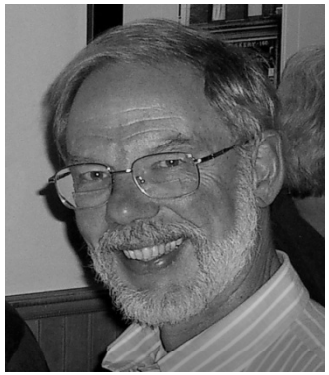
Dr. Angela K. Wilson, Co-Director, **CASCaM**

Associate Professor of Chemistry
2003 NSF CAREER Award
2004 IJQC Young Investigator Award
2005 U.S. Chair for Chinese-American Frontiers of Science (National Academy of Sciences)



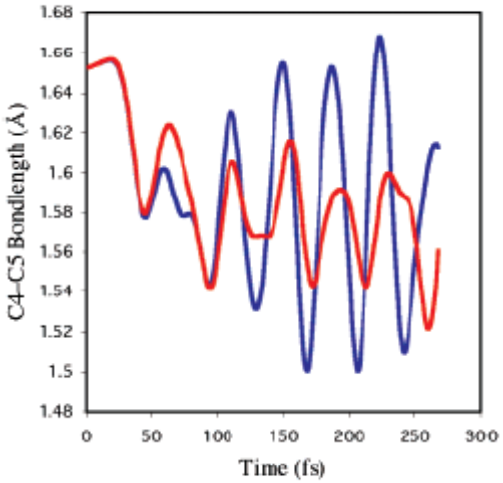
The Wilson group is a leader in the development of more accurate and efficient chemical modeling techniques.

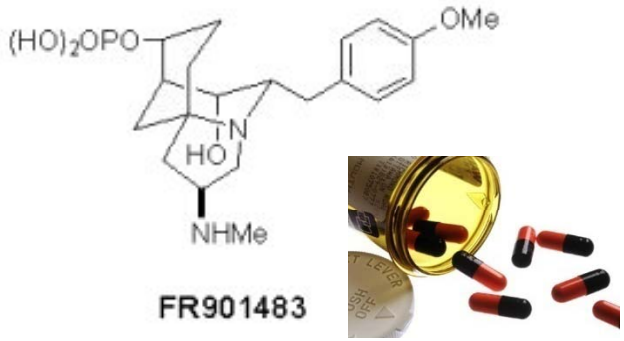
Current Funding Sponsors



Dr. Weston T. Borden

Robert A. Welch Chair of Chemistry
2005 Cope Scholar Award, American Chemical Society
Associate Editor, Journal of the American Chemical Society





http://www.musc.edu/hrm/images/public/pills.jpg

Modeling is a window on species too unstable or processes too fast to be studied by experiment. Such insight leads to useful products.

Current Funding Sponsors

Center for Enabling New Technologies through Catalysis

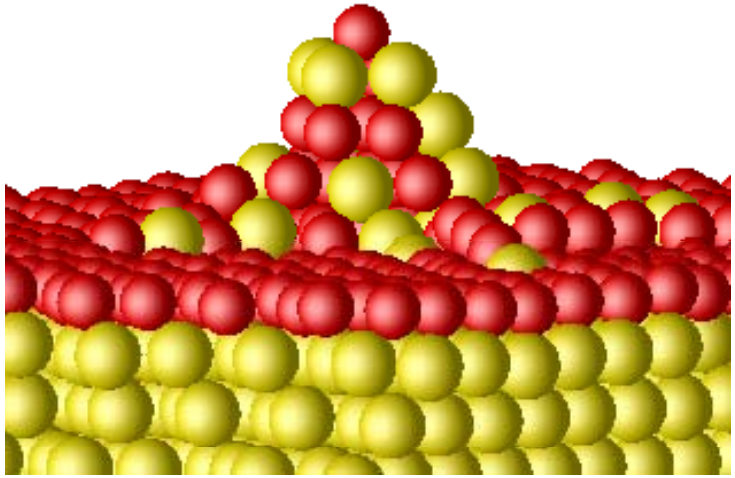
NSF

THE Welch FOUNDATION

Dr. Paul S. Bagus

Research Professor of Chemistry
Editorial Board, Journal of Electron Spectroscopy
Alexander von Humboldt Fellow

Nanomaterials



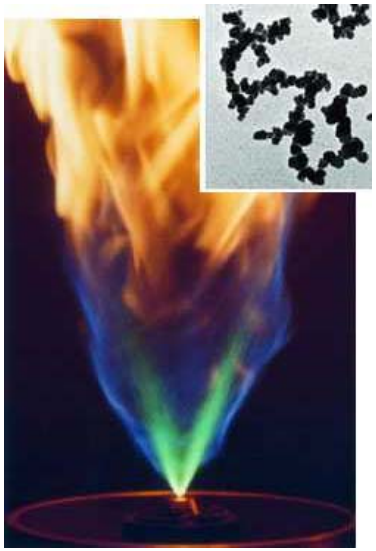
Using computer clusters to understand atomic metal clusters.

Current Funding Sponsors

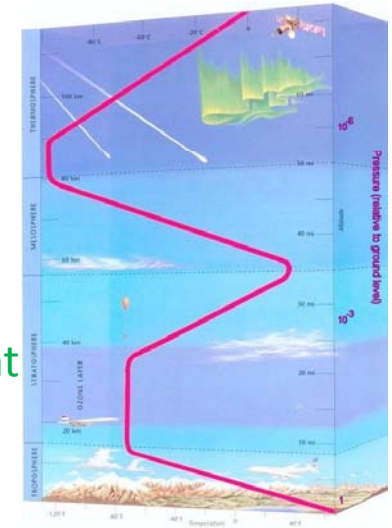
Dr. Paul Marshall

Regents Professor of Chemistry

Modeling fast chemical reactions is crucial in understanding combustion chemistry.



Chemistry in the atmosphere is difficult to study without scientific modeling.

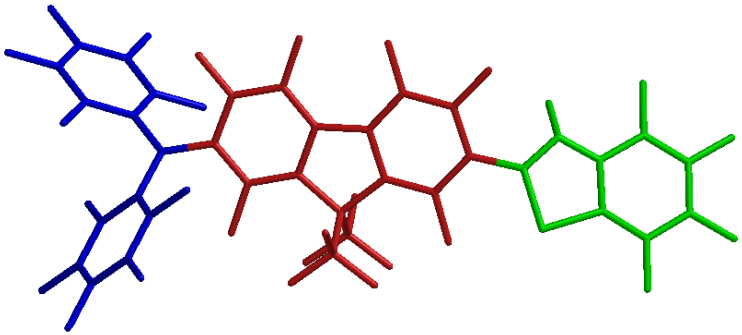


"Hot" chemistry: Combustion, flame-retardant materials, global warming.

Current Funding Sponsors

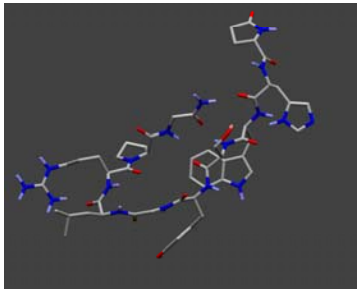
Dr. Martin Schwartz

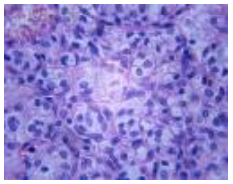
Regents Professor of Chemistry



TPA dye developed by USAF scientists.

Cetrorelix: A cancer hormone antagonist





Cancer cell

Developing novel electronics and medical materials.

Current Funding Sponsors

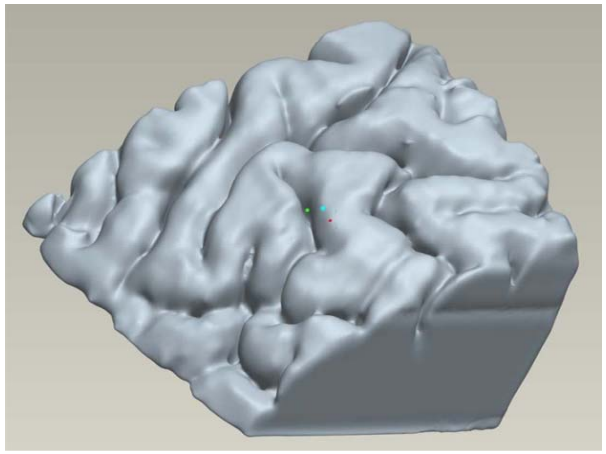
THE Welch FOUNDATION

AIR FORCE RESEARCH LABORATORY

Dr. Sandra Boetcher

Assistant Professor of Mechanical & Energy Engineering

Research interests include natural convection, biomedical heat transfer and fluid flow, and energy-related fields. Dr. Boetcher has collaborations to study epileptic brain cooling and laser tissue welding with IMTEC, a 3M Company (a biomedical company) and the University of Oklahoma.



Model of brain cooling. Courtesy IMTEC.

Current Funding Sponsors

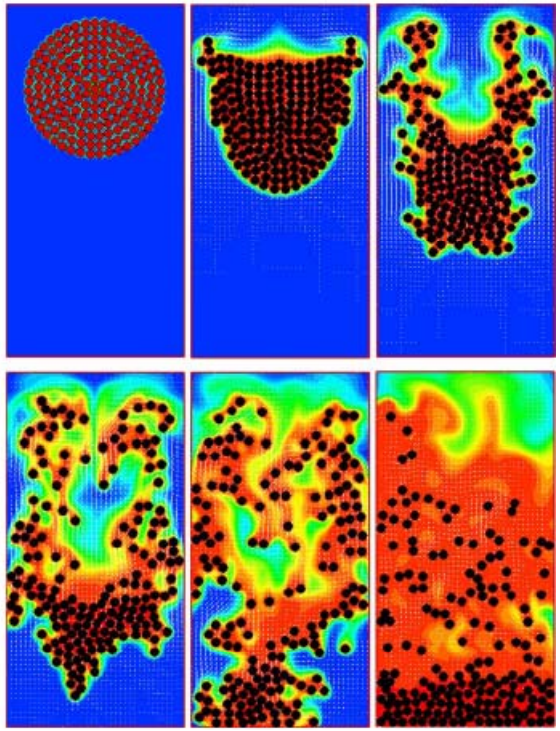
IMTEC® 3M a 3M Company

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

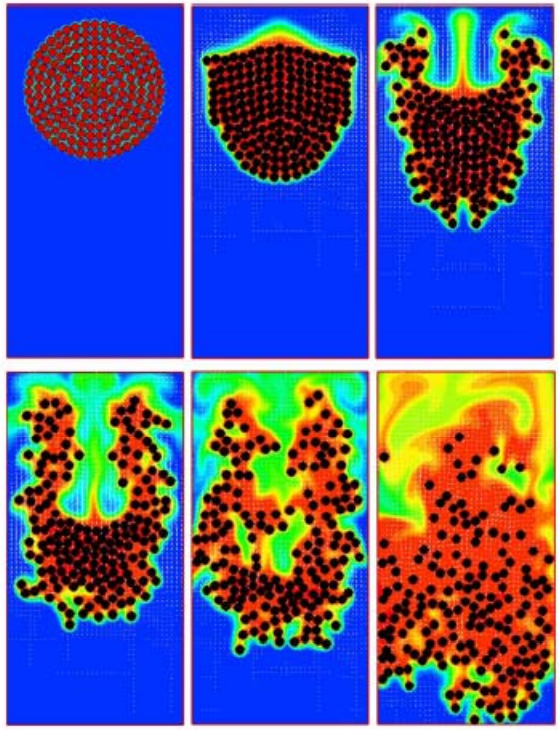
Dr. Zhi-gang Feng

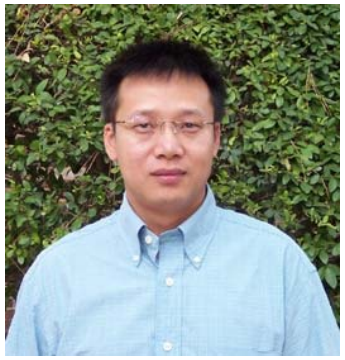
Assistant Professor of Materials Science and Engineering

Research interests: Modeling of turbulence and particulate flow, computational fluid dynamics.



Effect of buoyancy and viscosity on sedimentation of particles in a fluid

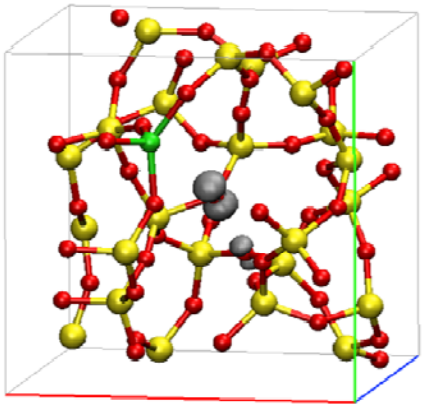




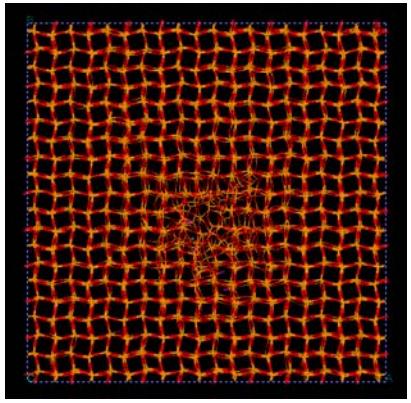
Dr. Jincheng Du

Assistant Professor of Materials Science and Engineering

Research interests: atomistic modeling of structure and dynamics of amorphous systems, *ab initio* calculations of materials surfaces, interfaces, and heterogeneous catalysts, electronic structure and phase transitions for ceramic oxides, classical and ab initio simulation of glass structure and properties



Model of dislocation in radiation damaged metal-oxide



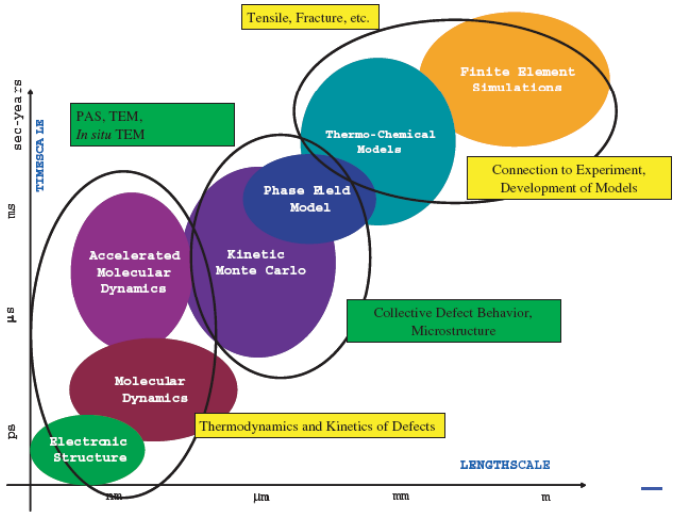
Simulation of the displacement cascade in cristobalite during erbium implantation

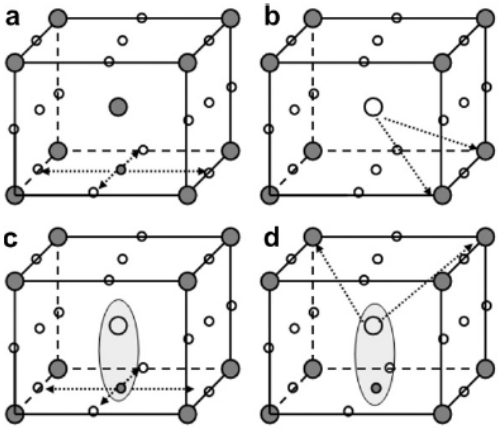
Current Funding Sponsors

Dr. Srinivasan Srivilliputhur

Assistant Professor of Materials Science and Engineering
Editorial Board of Review, Metallurgical and Materials Transactions
NSF CAREER Awardee

Research interests: Large-scale computer simulations of material failure, deformation and failure of materials in the presence of complex chemical reactions, new energy research, corrosion.





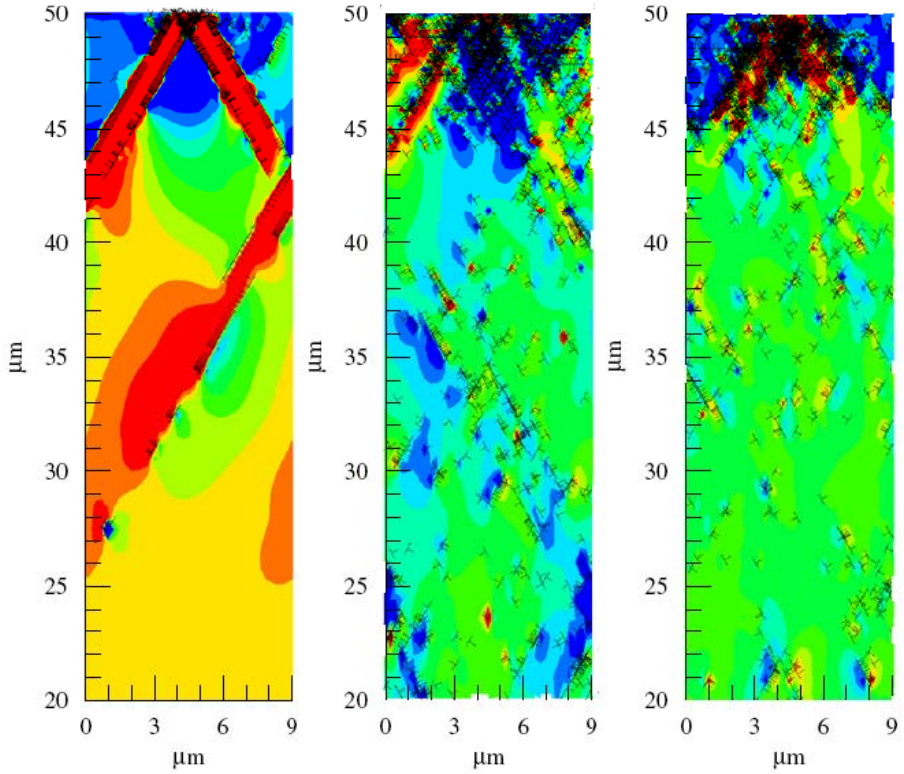
Model of He "bubble" formation in single crystal bcc Fe

Current Funding Sponsors

Dr. Alan Needleman

Professor of Materials Science and Engineering
Member, National Academy of Engineering

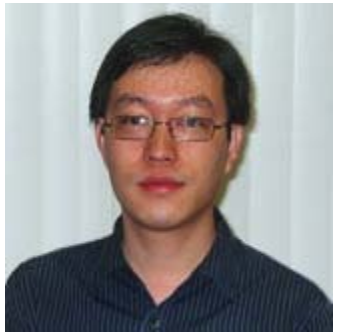
Research interests: Computational modeling of deformation and fracture processes in materials over a range of size scales from the nano to the macro.



Effect of indentation on surface and bulk stress and dislocation

Current Funding Sponsors

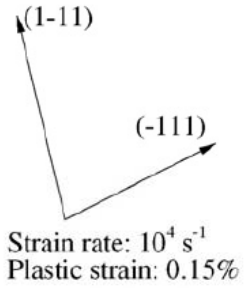
AIR FORCE RESEARCH LABORATORY

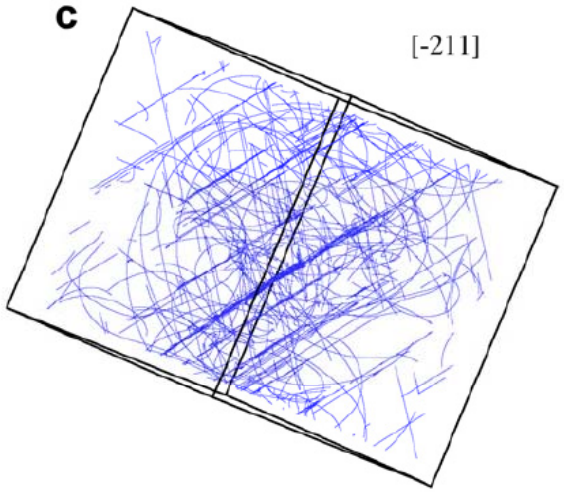


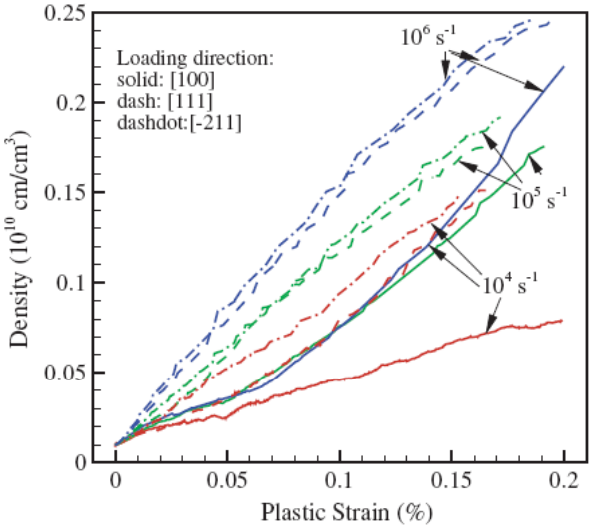
Dr. Zhiqiang Wang

Assistant Professor of Material Science Engineering

Research interests: Mesoscale Modeling & Dislocation Dynamics





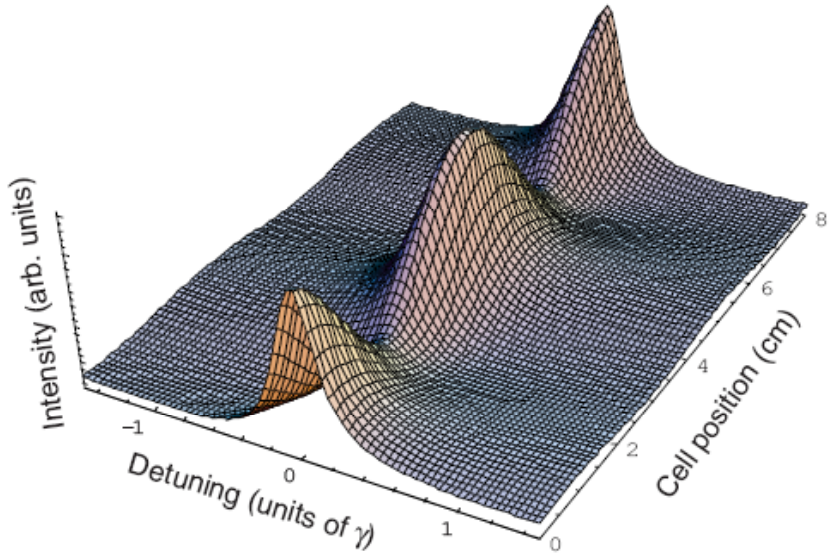


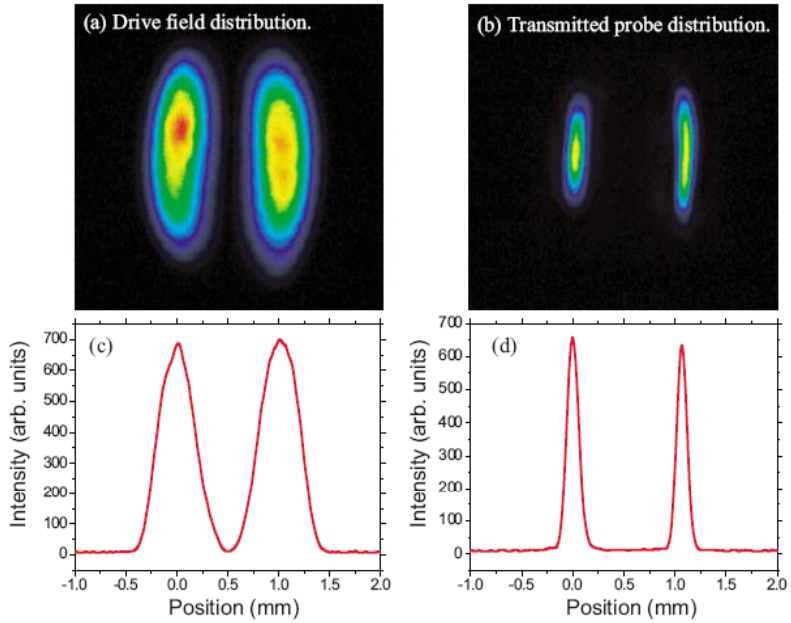
Mesoscale modeling
of defects
in fcc
crystal

Dr. Yuri Rostovtsev

Assistant Professor of Physics

Research interests: Condensed Matter Theory, Quantum Optics





CASCaM = Collaborative

- Inside/outside UNT
- Other centers of excellence in modeling
- Theory + experiment
- With national lab and industrial partners

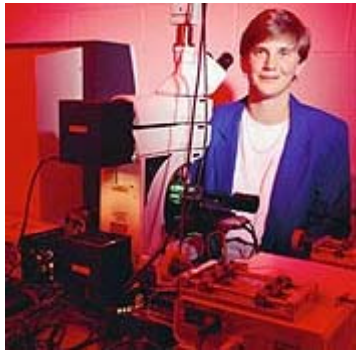
NSF Chemical Bonding Center
CENTC

Center for Enabling New Technologies through Catalysis

CENTC is first Phase II CBC; CASCaM is providing modeling expertise and training

The $15 million grant to the Center for Enabling New Technologies through Catalysis will continue to foster research to find easier and better ways of manipulating strong chemical bonds found in most materials.

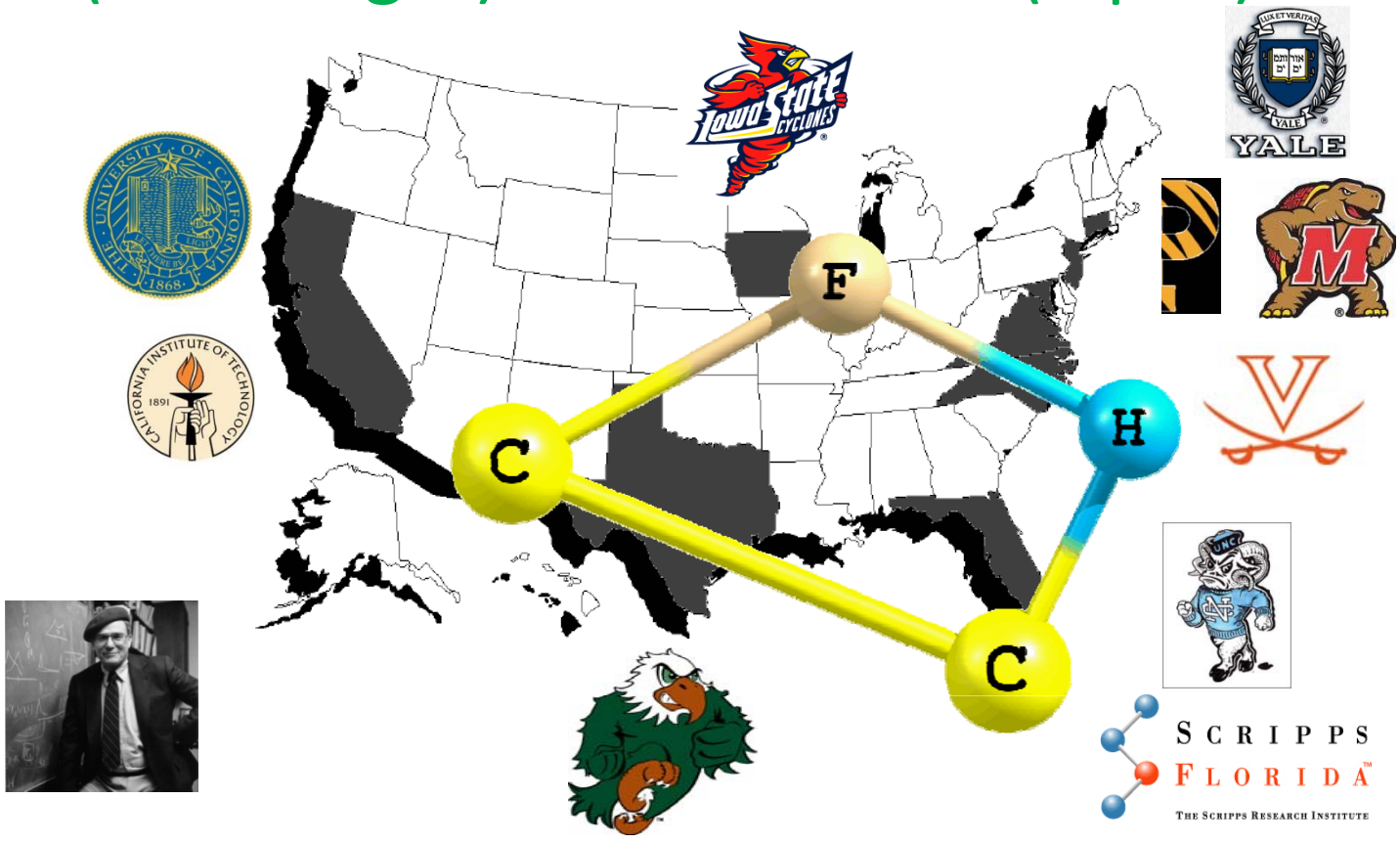
Lockheed Nanotechnology Group



- Multi-institutional NSF-CCI proposal submitted
- NSF-IMI: CHiPS(NCSU)+CASCaM(UNT)

Center for Catalytic Hydrocarbon Functionalization

- Goal: Viable catalyst to convert methane (natural gas) into methanol (liquid)

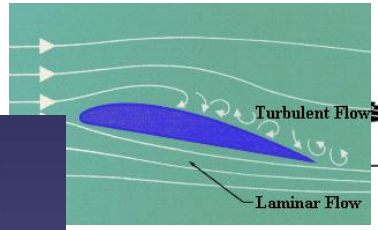


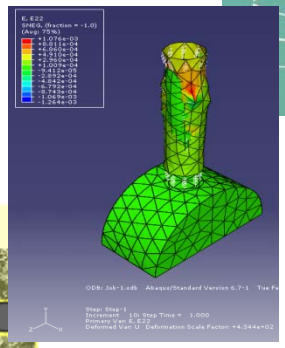
1 of 40 EFRCs

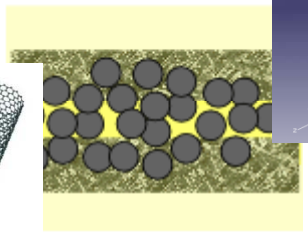
Comp Teams
- Goddard (CalTech)
- CASaM (UNT)

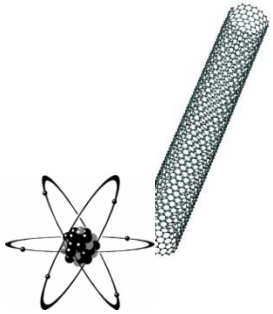
UNT Team
- Cundari
- Du
- Srivilliputhur

Project ISES



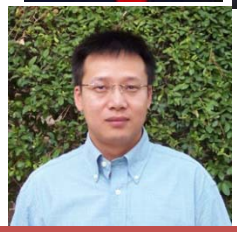






Time Scale

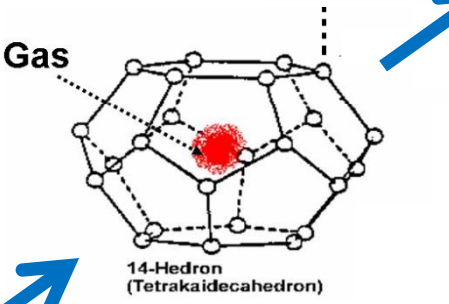
Length Scale

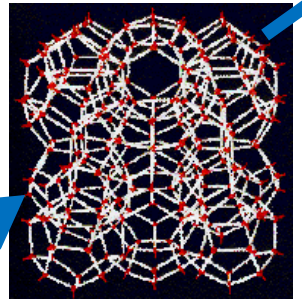


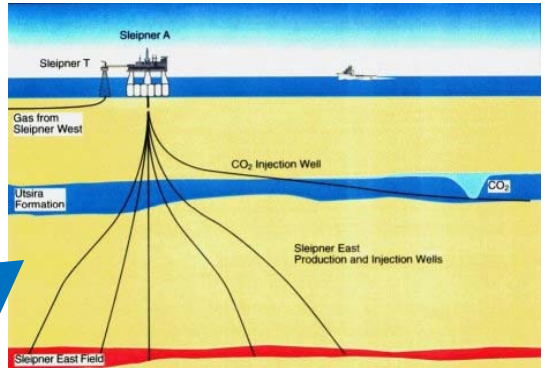
Modeling aerospace materials from continuum to atomic, closely interfaced with leading-edge characterization via UNT's CART

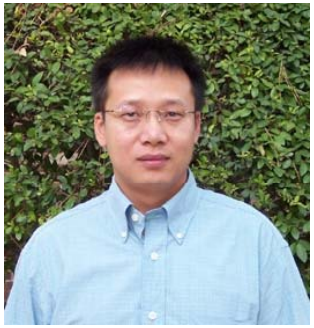
Multi-scale Modeling of CO_2 Storage

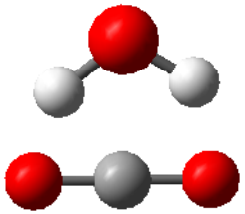
UNT UNIVERSITY OF NORTH TEXAS









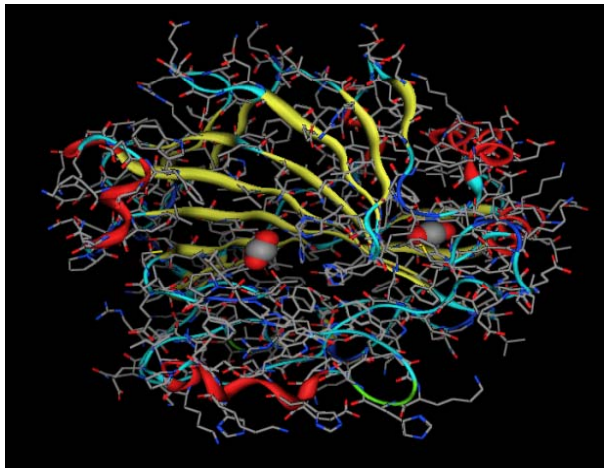


Time Scale

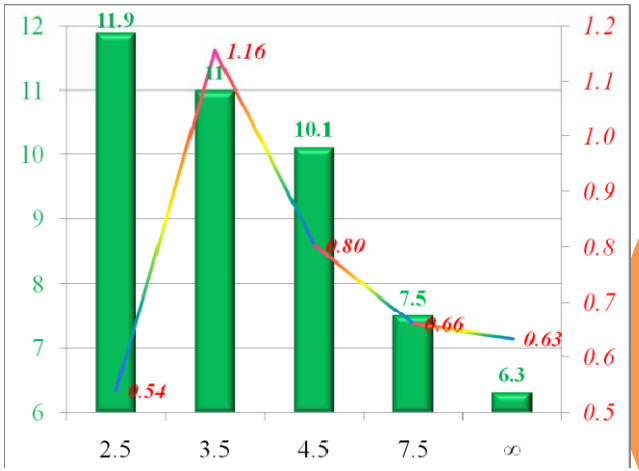
Length Scale

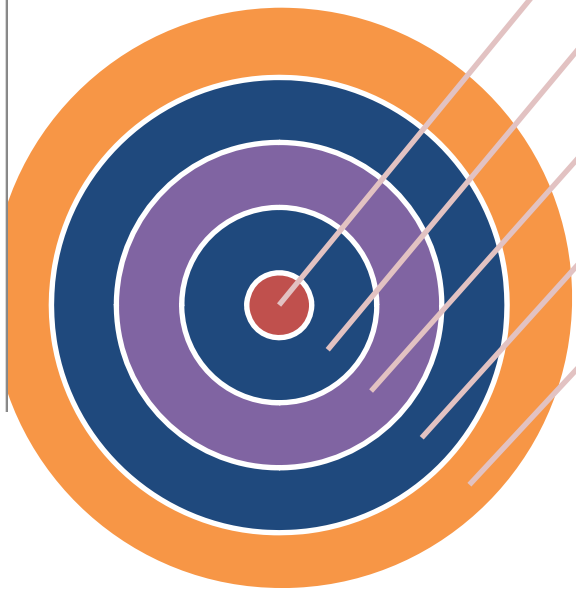
Modeling from a high-level ab initio simulation of a single CO_2/H_2O pair to CFD modeling of CO_2 in aqueous brines

CO_2-formatics



- Coupling bioinformatics tools & traditional comp chem methods to CO_2/protein binding
- Can we develop novel, bioinspired strategies for CO_2 sequestration?





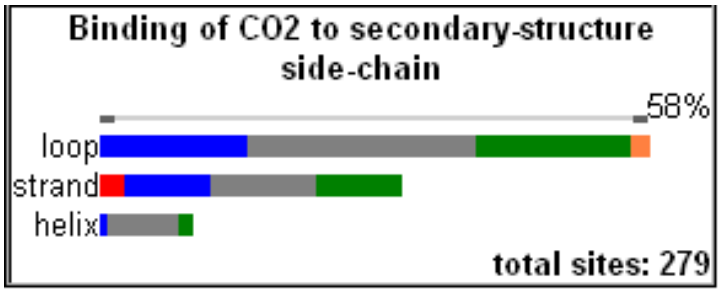
Carbon dioxide

"Direct" chemistry

Active site

Secondary structure

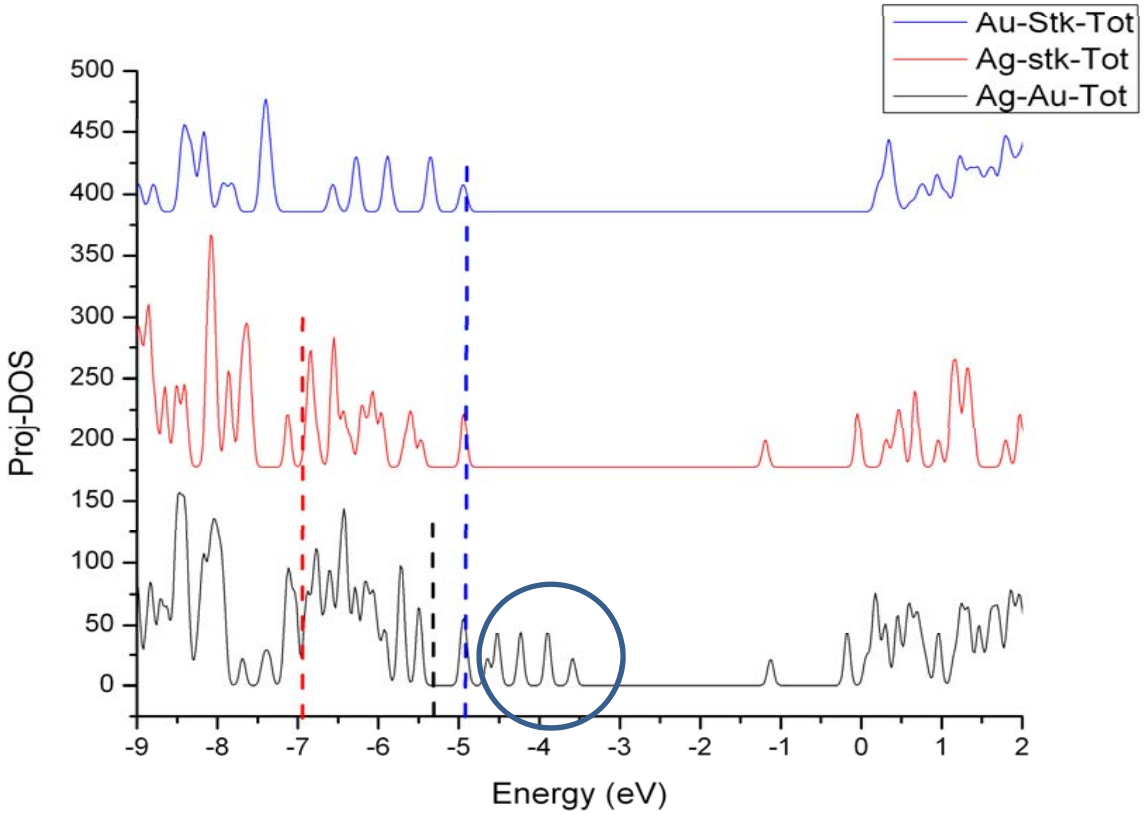
Enzyme

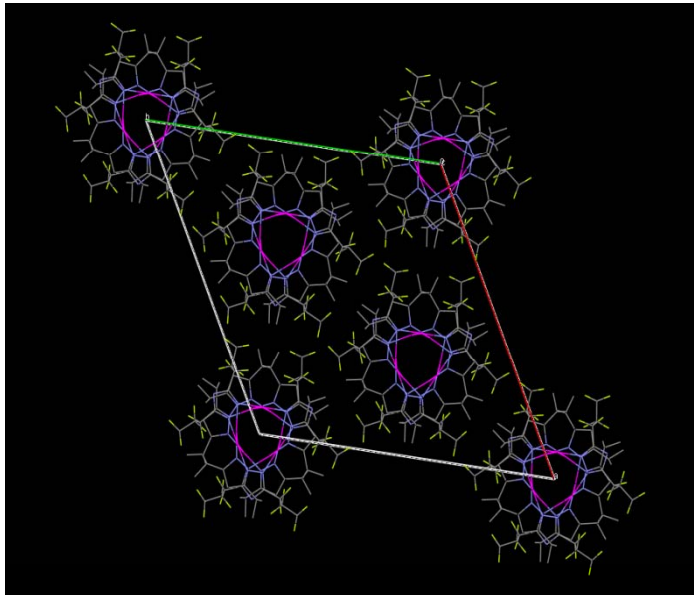


Joint DOE-BER Grant to Wilson & Cundari

Designer Electronics

- "Flexible" electronics for next-generation apps
- Joint NSF-DMR grant to design (Cundari, Du), synthesize (Omary) & construct (Gnade, UTD) flexible electronics





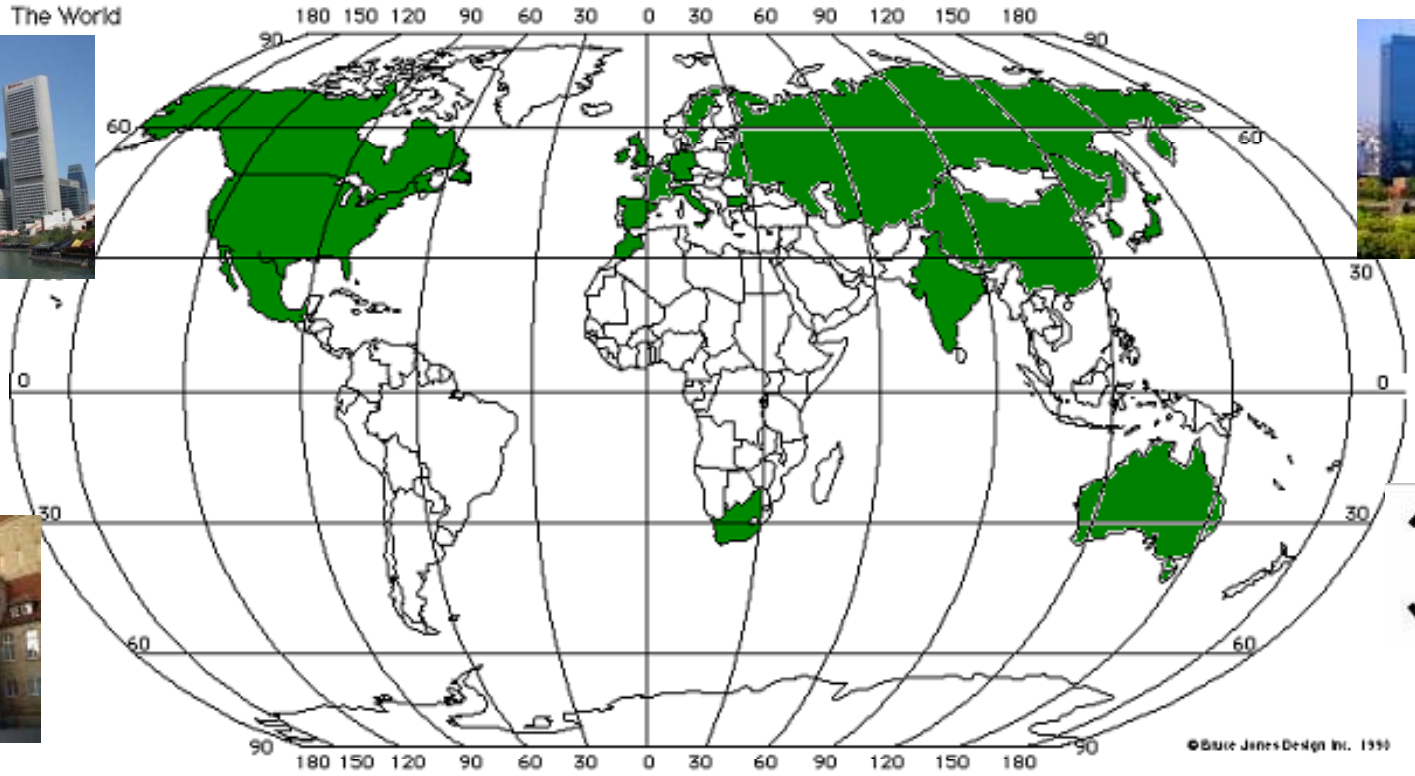
CASCaM = Diversity of Experience

Ian Haken
- **CASCaM** Research Student
- Intel Finalist
- Developed improved schemes for molecular “fingerprinting”

Paul Bagus
CASCaM Research Professor
- Pioneer
- Developed first practical computational chemistry program

CASCaM = Today’s Pioneers + Tomorrow’s Scientific Leaders

CASCaM Across the Globe



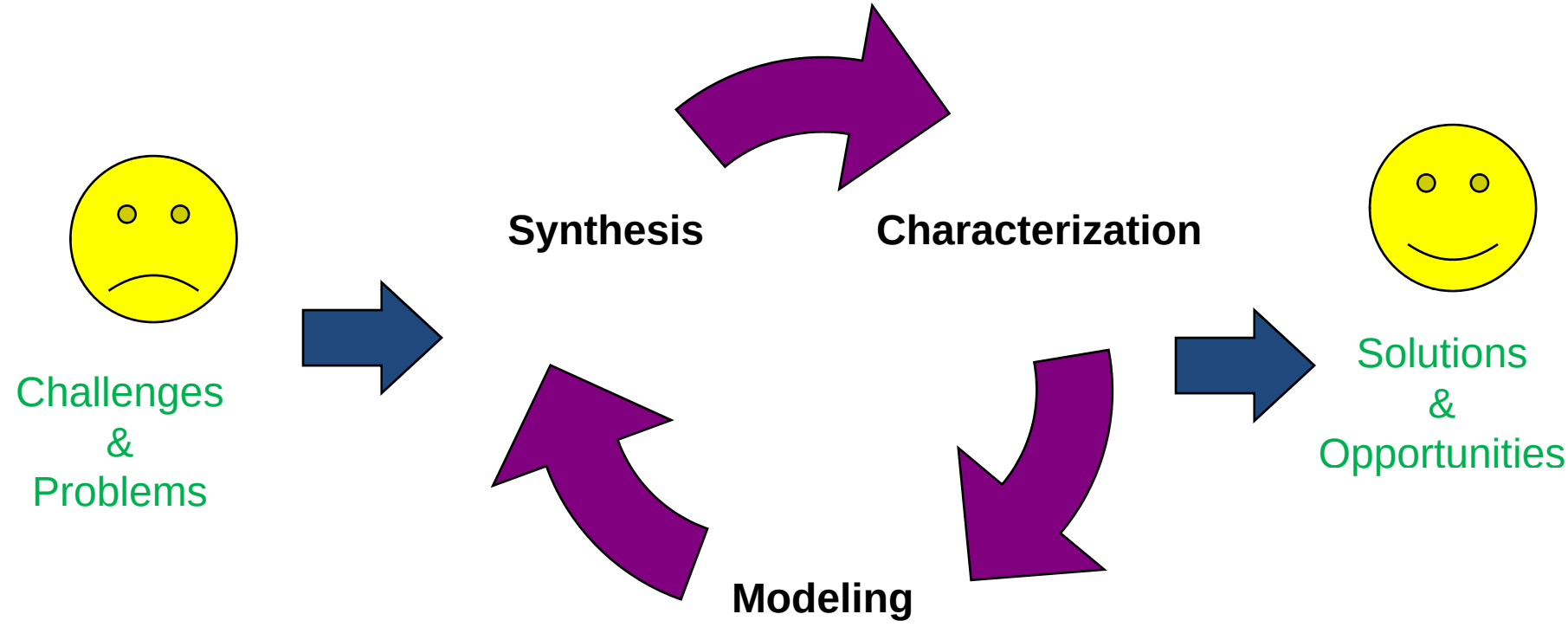
CASCaM = A Global Resource for Modeling Excellence

CASCaM Expertise

- ***Diversity of Chemistry***
  - Inorganic/Organometallics
  - Organics
  - Materials Chemistry
  - Biological Chemistry
  - Physical Chemistry
- ***Diversity of Methodology***
  - Molecular mechanics
  - Semiempirical quantum mechanics
  - Ab initio & density functional theory
  - Bioinformatics
  - Artificial intelligence
  - Molecular dynamics

Diversity Of Experience = Greater Employment Potential!

The CASCaM Ethos



- Both on- and off-campus, CASCaM focuses on the integration of cutting-edge theory and simulation, integrated with experiment and characterization to provide comprehensive solutions to technical problems

Hiring Plan

Five – seven (5-7) faculty hires over next 3 years

- Junior and senior faculty hires
- Focus areas of application
  a) Aerospace materials
  b) Biomaterials
  c) Catalysis

- Goals for hiring
  - Fill in “gaps” in modeling expertise: time/length scales & methodologies
  - Diversify expertise base: applications, development, theory, coding
  - Complement on-campus experimental strengths

Targeted Hire Areas

Modeling of materials interfaces/surfaces

- 1 senior hire

Multi-scale/multi-physics materials modeling

- 1 senior hire

Mesoscale/microstructure evolution

- 1 junior hire

Continuum scale lifetime prediction

- 1 junior hire, 1 senior hire

Informatics

- 1 senior hire

Computational Chemistry

- 1 senior hire (2008)

Additional Staff

- 1 ➔ Visualization, programming, code development, *etc*.
- 1 ➔ administrative assistant ➔ PR, recruiting, outreach, dissemination, *etc*.

CASCaM Facilities

- **Over 3,000 sq ft. of server rooms within the chemistry building**
- **Over 2,000 cores (5 Teraflops) housed in the chemistry building devoted to computational chemistry research**

- **Ph.D.-staff member to manage computational chemistry facilities and provide training**
- **Computational Chemistry Instructional Facility (CCIL)**

- **UNT's Center for Advanced Scientific Computing and Modeling (CASCaM) is expanding and will invest in ~5,000 cores in 2009-2010 → ca. $1.5M.**
- **Computational chemistry faculty also heavily use other facilities – UNT's Research Faculty clusters, National TeraGrid facilities, and DOE ("Grand Challenge") facilities.**

Timeline*

Year 0

- Start renovation
- 1st installment of new UNT research computing facility
- Computational chemistry senior hire

Year 1

- Continue renovation
- 2nd installment - computing facility
- Junior hire – Mesoscale modeling
- Senior hire – Multiscale modeling

Year 2

- Complete renovation
- Junior hire – Continuum modeling
- Senior hire - Informatics
- 3rd installment – computing facility

Year 3

- Senior hire –Surfaces/Interfaces modeling

•Timeline is tentative and for illustrative purposes; flexibility in hiring will be key;

• Year 0 = 2008 – 2009

Summary

- ✓ Hires will build upon existing expertise @ UNT
  - Expertise across many applications areas
  - Expertise across many time/length scales
  - 5 -7 faculty hires, next 2 – 3 years
- ✓ Core faculty are highly collaborative
  - Modeling and expt
  - Modeling and modeling
- ✓ Upgrades to infrastructure &equipment

Make UNT a recognized leader in
cross-disciplinary materials modeling research