

**THURSDAY, FEBRUARY 7, 2002
EMBASSY SUITES**

REGISTRATION 8:00-8:30

B. V. McKoy (Caltech), Chairperson

L. Davis (HPCMO - Department of Defense) 8:30-9:00
*DoD HPC Modernization Program in 2002:
Moving DOD Computational Science Forward*

E. Carter (University of California, Los Angeles) 9:00-9:30
Nanoscope Origins of Materials Failure

A. Nakano (Louisiana State University) 9:30-10:00
*Scalable Algorithms and Parallel Computing
Framework for Multiscale Materials Simulations
Beyond Teraflop*

COFFEE BREAK 10:00-10:30

S. S. Iyengar (Louisiana State University), Chairperson

R. Roskies (Pittsburgh Supercomputing Center) 10:30-11:00
Terascale Computing at PSC

J. J. Dongarra (University of Tennessee) 11:00-11:30
*High Performance Computing, Computational
Grid, and Numerical Libraries*

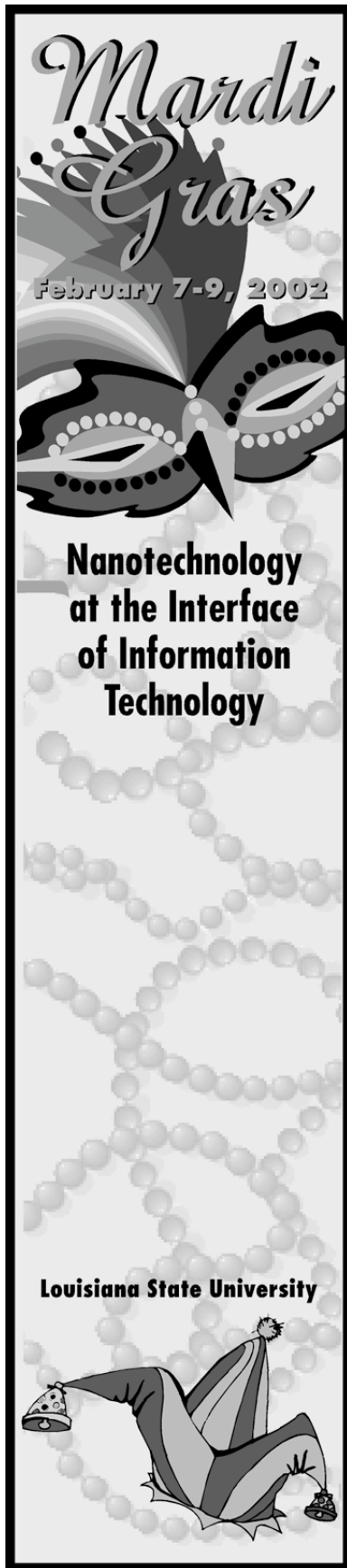
D. E. Keyes (Old Dominion University) 11:30-12:00
Terascale Optimal PDE Solvers

LUNCH BREAK 12:00-1:15

S. W. de Leeuw (Delft University, Holland), Chairperson

W. Wilson (Eglin Air Force Research Laboratory) 1:15-1:45
*Air Force Research in Nanoenergetics -
Potential Advantages and Challenges*

T. D. de la Rubia (Lawrence Livermore Nat'l Lab) 1:45-2:15
*Strength and Plasticity in Nanocrystalline Cu
and Ni - Atomic Scale Simulations and
Experimental Observations*



M. Baskes (Los Alamos National Laboratory) 2:15-2:45
Atomistic Simulations of the Plasticity Behavior of Single Crystal and Polycrystalline Metals

L. Manna (University of California, Berkeley) 2:45-3:15
Inorganic Nanocrystals and Nanorods: Synthesis and Biological Applications

S. Kodiyalam (Louisiana State University) 3:15-3:45
Grain Boundaries in Gallium Arsenide Nanocrystals

COFFEE BREAK 3:45-4:15

P. Russo (Louisiana State University), Chairperson

A. Pechenik (Cornell University) 4:15-4:45
Nanofabrication Research and Capabilities at Cornell Nanofabrication Facility

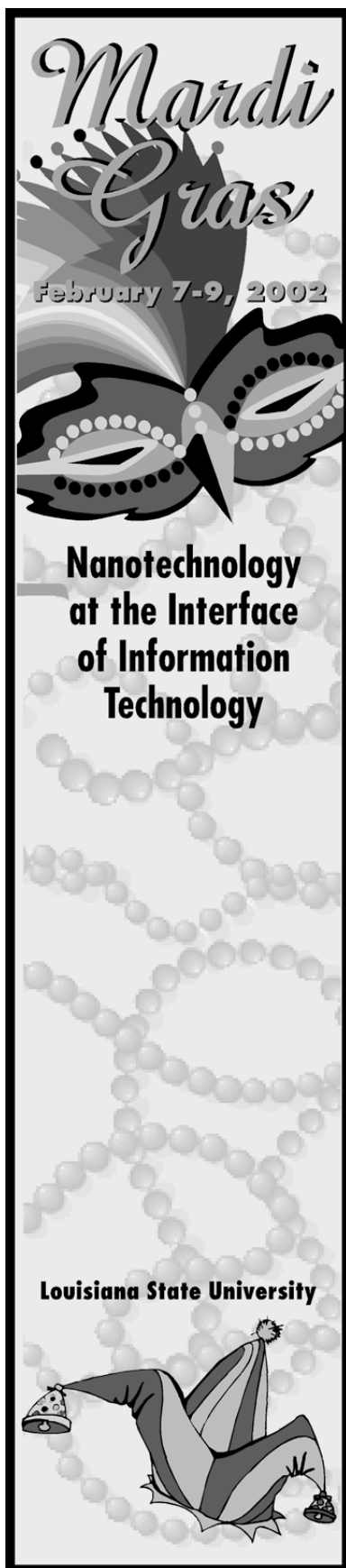
M. Jaffe (New Jersey Institute of Technology) 4:45-5:15
Process-Structure-Property Relationships of Polymeric Biomaterials

C. Massobrio (Institut de Physique et Chimie des Matériaux de Strasbourg, CNRS, France) 5:15-5:45
Short and Intermediate Range Order in Disordered Ge_xSe_{1-x} Systems

H. Iyetomi (Niigata University, Japan) 5:45-6:15
Nanoscale Inhomogeneities in Multicomponent Oxide Glasses: Molecular Dynamics Simulation Study

COCKTAILS 6:15

DINNER 7:00



**FRIDAY, FEBRUARY 8, 2002
EMBASSY SUITES**

S. Acharya (Louisiana State University), Chairperson

D. Koelling (Department of Energy) 8:00-8:30
"Nano" and "Bio" at the Department of Energy

R. Siegel (Rensselaer Polytechnic Institute) 8:30-9:00
Directed Assembly of Functional Nanostructures

R. Armstrong (Eglin Air Force Research Lab) 9:00-9:30
Nanometric Aspects of Energetic Crystal Properties/Testing

COFFEE BREAK 9:30-10:00

R. Beuerman (LSU HSC), Chairperson

T. Wilson (Oxford University) 10:00-10:30
Adaptive Aberration Correction in Confocal Microscopy

J. Trent (NASA Ames Research Center) 10:30-11:00
The Use of 'Extremophile' Proteins in Bio-Nano-Technology

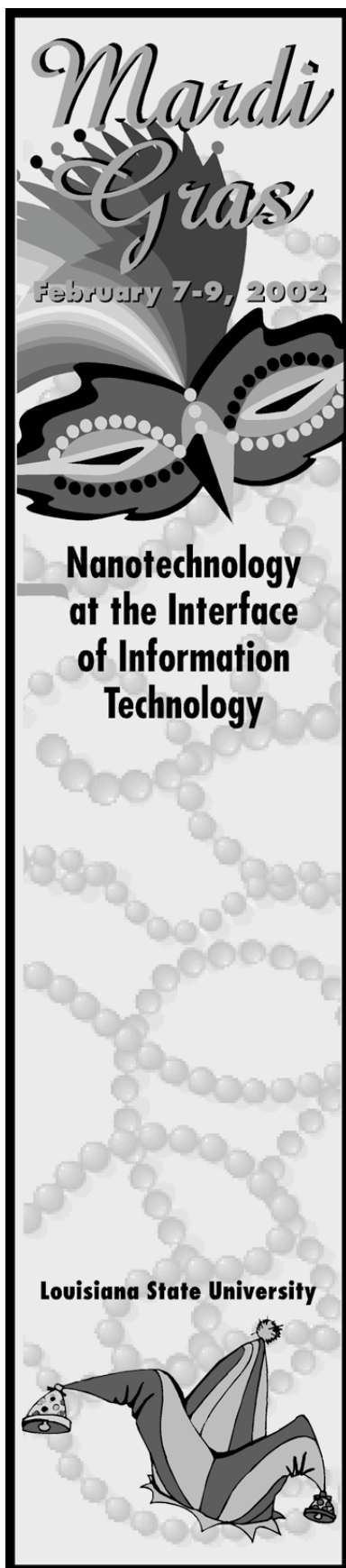
S. Lee (The Ohio State University) 11:00-11:30
The Convergence of Biology and Nanoscience: An Opportunity for Molecular Devices Built with Biological Molecules

V. Petrenko (Auburn University) 11:30-11:45
Phage as Engineered Self-Replicating Self-Assembling System for Nanofabrication of Bioselective Sensors

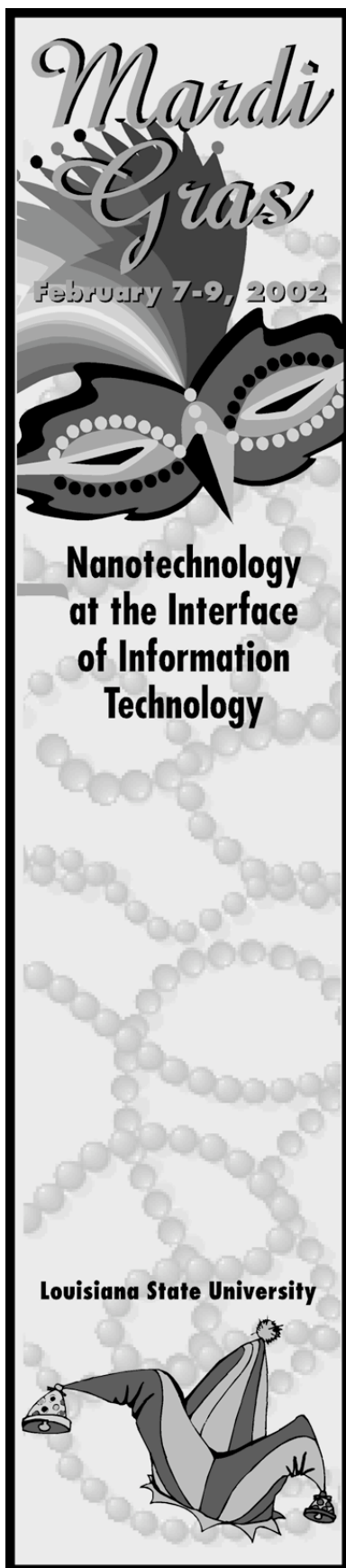
LUNCH BREAK 11:45-1:00

H. Silverman (Louisiana State University), Chairperson

J. T. Groves (University of California, Berkeley) 1:00-1:30
Pattern Formation and Cell Signaling at an Intermembrane Synapse



K. Reifsnider (Virginia Tech) <i>Physical Observation / Computational Structural Interfaces of Info-Bio-Nano Technology</i>	1:30-2:00
H. Jin (Louisiana State University) <i>High Resolution 3D Visualization of Atherosclerosis</i>	2:00-2:15
W. Dennis (University of Georgia) <i>Dynamical Processes in Green Fluorescent Protein</i>	2:15-2:30
COFFEE BREAK	2:30-3:00
T. Campbell (NAVO, Mississippi State Univ.), Chairperson	
G. S. Grest (Sandia National Laboratories) <i>Frictional Properties of Self-Assembled Monolayers</i>	3:00-3:30
M. Robbins (Johns Hopkins University) <i>Cracks and Crazes: From Molecular Simulations to the Macroscopic Toughness of Polymers</i>	3:30-4:00
S. M. Valone (Los Alamos National Laboratory) <i>United Atom Models of Polymeric Materials: A United Atomic Model of Polyethylene with the Modified Embedded Atom Method</i>	4:00-4:15
T. Soddemann (John Hopkins University) <i>Yielding PMMA - A Simulation Study</i>	4:15-4:30
M. Andrews (Texas A&M University) <i>An Overview of Magnetic Nano-Pinning at Texas A & M University</i>	4:30-4:45
A. Jalbout (University of New Orleans) <i>Monte Carlo Simulation on the RKKY Interactions of Co-Doped ZnO Film</i>	4:45-5:00
M. R. Geller (University of Georgia) <i>Quantum Energy Transport in Nanoscale Systems</i>	5:00-5:15



K. Patton (University of Georgia) 5:15-5:30
*Phonons in a Nanoparticle Mechanically Coupled
to the Environment*

CCLMS TOUR 5:45

BANQUET 7:00

**SATURDAY, FEBRUARY 9, 2002
EMBASSY SUITES**

R. Lipton (Louisiana State University), Chairperson

M. Meyyappan (NASA Ames Research Center) 8:30-9:00
*Carbon Nanotubes in Nanoelectronics and Sensor
Development*

P. Ajayan (Rensselaer Polytechnic Institute) 9:00-9:30
*Building Organized Architectures with Carbon
Nanotubes*

A. Svizhenko (NASA Ames Research Center) 9:30-9:45
*Effects of Structural Deformation in Chirality on
Electron Transport in Carbon Nanotubes*

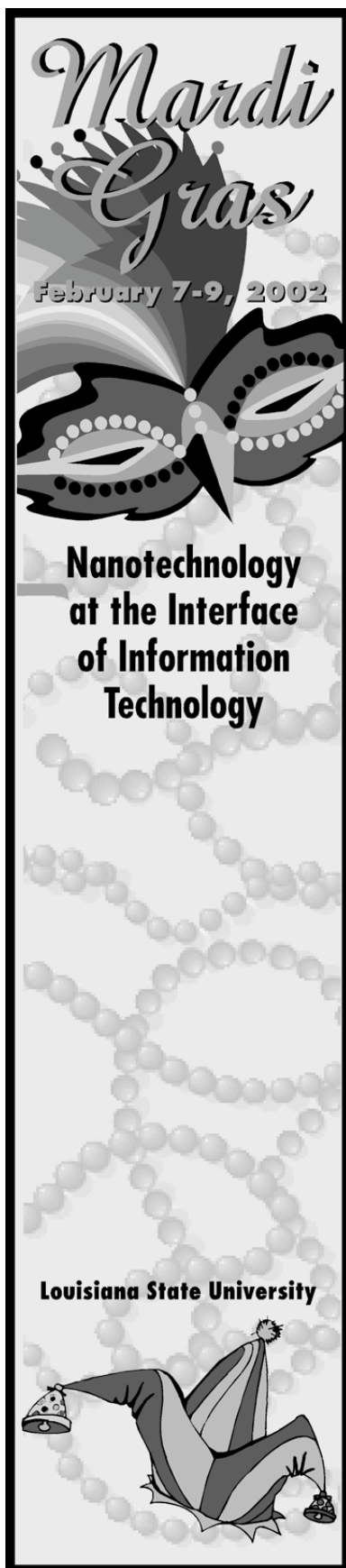
COFFEE BREAK 9:45-10:15

J. Chan (Louisiana State University), Chairperson

R. Car (Princeton University) 10:15-10:45
*Ab-initio Molecular Dynamics Studies of
Nanostructures and Biomolecules*

X. Su (Louisiana State University) 10:45-11:15
*InAs/GaAs Square Nanomesas: Multimillion-
Atom Simulations on Parallel Computers*

P. Cremer (Texas A&M University) 11:15-11:45
*Exploiting Nanofilm Coatings in Microfluidic
Devices for Biosensing*



P. Landon (University of Texas at Dallas) 11:45-12:00
Techniques for Guiding the Assembly of FCC, BCC, HCP, Tetragonal and Triclinic Photonic Crystals

LUNCH BREAK 12:00-1:15

W. J. Meng (Louisiana State University), Chairperson

R. Ritchie (Lawrence Berkeley National Lab) 1:15-1:45
A Mechanistic Evaluation of Mechanisms of "Near-Nanoscale" High-Cycle Fatigue Failures in Polysilicon Thin Films for MEMS

V. Prasanna (University of Southern California) 1:45-2:15
Cache-Conscious Algorithm Design

S. Shankar (Intel) 2:15-2:45
Self-Consistent Modeling of Weakly Ionized Plasmas - Challenges in Quantum and Classical Mechanics

H. Wong (Louisiana State University) 2:45-3:00
Coupled Grooving and Migration of Inclined Grain Boundaries

COFFEE BREAK 3:00-3:15

A. Nakano (Louisiana State University), Chairperson

Y. Saad (University of Minnesota) 3:15-3:45
Numerical Techniques for Time-Dependent Density Functional Theory

A. Selloni (Princeton University) 3:45-4:15
Ab Initio Studies of Surface Structure Reactivity

J. E. Devaney (NIST) 4:15-4:30
Parallelization and Visualization of Computational Nanotechnology LCAO Method

R. Schmieder (Nanologic, Inc.) 4:30-4:45
Nanologic: A Logical Bridge to Nanocomputing

TRIP TO NEW ORLEANS 5:15