

# EMERSON CENTER LECTURESHIP AWARD SYMPOSIUM

## Interface of Computers with Chemistry, Physics, Biology & Materials: Methods & Applications

Cherry L. Emerson Center for Scientific Computation, Emory University



Dr. Cherry L. Emerson

### Saturday, May 1, 2004

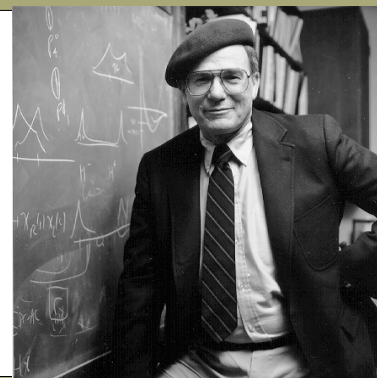
### Location: 360 Atwood Hall, Emory University

#### AWARD WINNER & KEYNOTE SPEAKER:

### William A. Goddard, III

Charles and Mary Ferkel Professor of Chemistry, Materials Science, and Applied Physics  
Director, Materials and Process Simulation Center (MSC), California Institute of Technology

We will highlight some recent advances in methodology and will illustrate them with recent applications to problems involving Proteins, DNA, Polymers, Ceramics, Metals, Semiconductors, and Catalysis. This lecture will have three parts: (1) strategy and tactics in applications of the methods to a range of practical problems involving materials science, catalysis, and nanotechnology; (2) recent advances in protein folding and drug design with applications to structure and function of Protein Coupled Receptors (GPCRs), including the receptors for smell, taste, dopamine, epinephrine, histamine, and pain, and (3) details of methods used in the applications presented in Parts 1 and 2.



#### INVITED SPEAKERS:

#### SCHEDULE OF EVENTS:



**Stefan Boettcher**  
Dept. of Physics, Emory University, Atlanta



**Rigoberto Hernandez**  
School of Chemistry & Biochemistry, Georgia Tech., Atlanta



**James Kindt**  
Dept. of Chemistry, Emory University, Atlanta



**Jamal Musaev**  
Emerson Center, Emory University, Atlanta



**Steven J. Stuart**  
Dept. of Chemistry, Clemson University, Clemson

9:30 - 9:50

WELCOME & AWARD PRESENTATION

9:50 - 11:00

Prof. William Goddard (CalTech, California), *De Novo Multi-Scale Simulations Applied to Materials (Polymers, Ceramics, Metals, Semiconductors), Catalysis, Proteins, and DNA*

11:00 - 11:50

Prof. James Kindt (Emory Univ., Georgia), *Molecular and Mesoscale Modeling of Membranes*

11:50 - 1:30

LUNCH (and tour of Emory and Emerson Center)

1:30 - 2:20

Prof. R. Hernandez (Georgia Tech., Georgia), *The Role of the environment in Dense Polymerization, Protein Motion and Binding*

2:20 - 3:10

Dr. Jamal Musaev (Emory Univ., Georgia), *Computational Designing of Catalytic Processes: From the Transition Metal Cations and Clusters through Organometallic Complexes to Enzymes*

3:10 - 3:30

COFFEE BREAK

3:30 - 4:20

Prof. Steve Stuart (Clemson Univ., S. Carolina), *Bond-Order Approaches for Reactive Materials Science Simulations*

4:20 - 5:10

Prof. Stefan Boettcher (Emory Univ., Georgia), *Low-Energy Excitations in Very Large Hyper-cubic Spin Glasses in  $d=3$  to  $d=7$*

5:10

Closing

6:00 - 8:30

DINNER (by invitation only)

#### REGISTRATION AND CONTACT INFORMATION:

Email: [clec@euch4e.chem.emory.edu](mailto:clec@euch4e.chem.emory.edu)

<http://www.emerson.emory.edu/local/register.html>

1515 Dickey Drive, Atlanta, GA 30322

Phone: 404-727-2380; Fax: 404-727-7412

Registration is free, but you must register to attend.

The Emerson Center Lectureship Award was established in fall 2003 to recognize distinguished achievements by scientists in computational sciences and to facilitate collaboration among different disciplines of computational sciences. On the board of the Emerson Center Lectureship Award Selection Committee are Professors Kurt Warncke (Physics, chair), Rustom Antia (Biology), Michele Benzi (Math & Computer Science), Justin Gallivan (Chemistry), Keiji Morokuma (Emerson Center), and Keith Wilkinson (Biochemistry) of Emory University. Dr. Jamal Musaev (Emerson Center) is appointed as the Lectureship Coordinator.



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