new faces on the
forefront of research

QTP

quantum theory project

NEWS FALL 2006

UF

on the cover

The Quantum Theory Project is pleased to announce the addition of three new faculty members. They are, left to right, **So Hirata** (Assistant Professor, Chemistry), **Adrian Roitberg** (Associate Professor, Chemistry) and **Kennie Merz** (Professor, Chemistry). So's research includes the development of an artificial intelligence system to implement new chemical theories. Adrian's interests include accurate calculations of biological systems via quantum mechanics, statistical mechanics and molecular dynamics. Kennie's research combines quantum mechanics with molecular mechanics to study large biological systems and to design new drugs.

meet our faculty

Rodney J. Bartlett
Coupled-Cluster Theory, Theoretical Molecular Spectroscopy, Polymers

Hai-Pin
Electronic
Properties
Hydrolyti
Materials
Interacti

Since its founding in 1960 by Professor Per Olov Löwdin, the Quantum Theory Project has grown into the world's largest academic group in computational and theoretical chemical physics and quantum chemistry.

Working across the traditional boundary between Physics and Chemistry, we are a group of faculty and researchers dedicated to theoretical developments in quantum mechanics.

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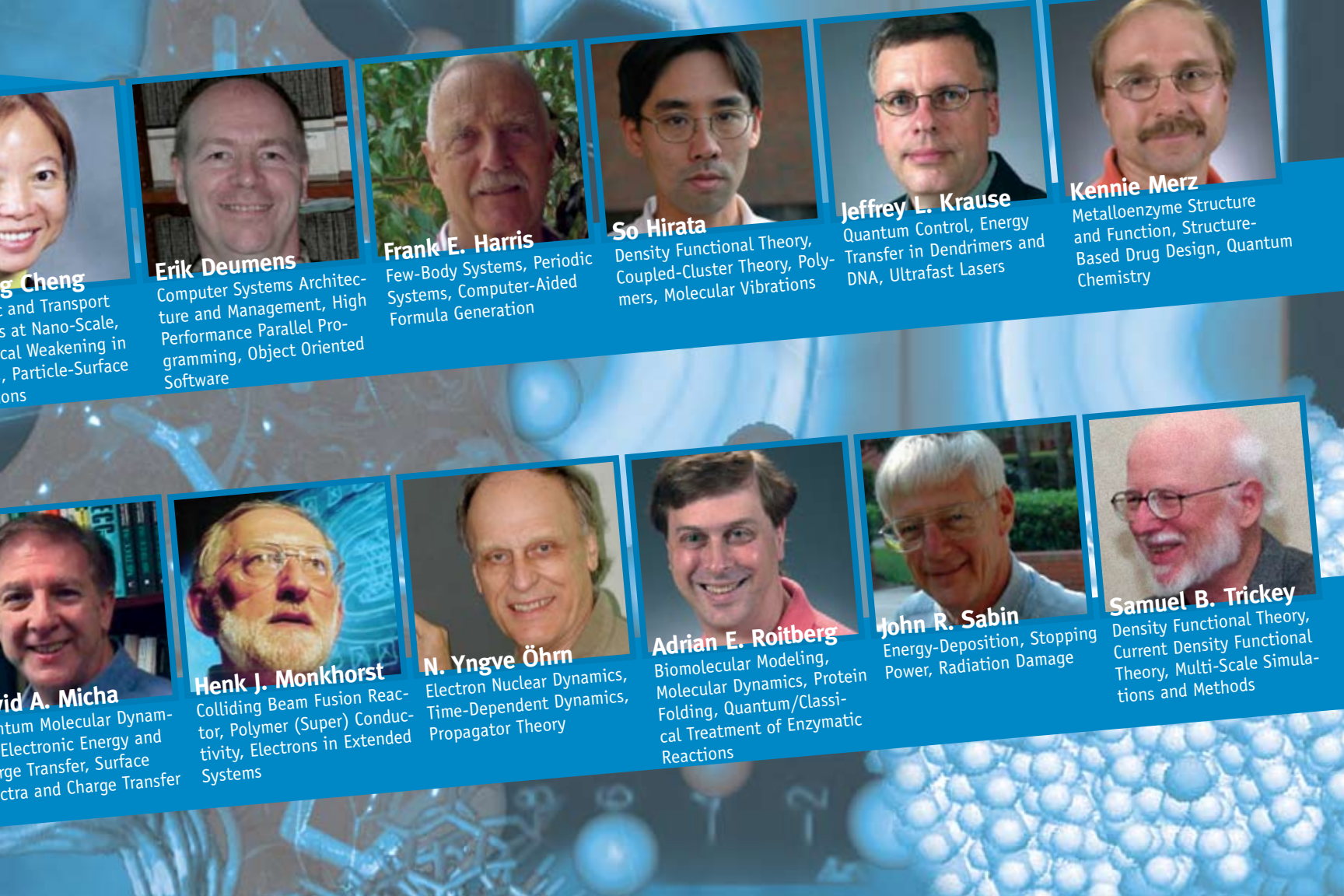

g Cheng
c and Transport
s at Nano-Scale,
cal Weakening in
, Particle-Surface
ons

Erik Deumens
Computer Systems Architecture and Management, High Performance Parallel Programming, Object Oriented Software

Frank E. Harris
Few-Body Systems, Periodic Systems, Computer-Aided Formula Generation

So Hirata
Density Functional Theory, Coupled-Cluster Theory, Polymers, Molecular Vibrations

Jeffrey L. Krause
Quantum Control, Energy Transfer in Dendrimers and DNA, Ultrafast Lasers

Kennie Merz
Metalloenzyme Structure and Function, Structure-Based Drug Design, Quantum Chemistry

vid A. Micha
ntum Molecular Dynam-
Electronic Energy and
rge Transfer, Surface
ctra and Charge Transfer

Henk J. Monkhorst
Colliding Beam Fusion Reactor, Polymer (Super) Conductivity, Electrons in Extended Systems

N. Yngve Öhrn
Electron Nuclear Dynamics, Time-Dependent Dynamics, Propagator Theory

Adrian E. Roitberg
Biomolecular Modeling, Molecular Dynamics, Protein Folding, Quantum/Classical Treatment of Enzymatic Reactions

John R. Sabin
Energy-Deposition, Stopping Power, Radiation Damage

Samuel B. Trickey
Density Functional Theory, Current Density Functional Theory, Multi-Scale Simulations and Methods

Greetings from the Quantum Theory Project at the University of Florida!

We are an interdisciplinary group in Chemistry and Physics dedicated to theoretical developments in quantum mechanics and their applications to atoms, molecules, materials and extended systems. As can be seen in the picture above, we are a large, diverse group, with 13 faculty and 50–60 students, visitors and postdocs. Each year, we organize and host the annual Sanibel Symposia, a preeminent gathering of international theorists. The 47th Symposium will be held February 22–27, 2007.

Please visit our web site at www.qtp.ufl.edu for more information or contact any of the faculty via email. Our addresses are all "lastname"@qtp.ufl.edu. Inquiries from prospective graduate students are especially welcome.

For the faculty,
Jeff Krause, QTP Director

Become a Friend of QTP– You Can Make a Difference!

QTP depends on your gifts to support the Sanibel Symposium, the Löwdin & Slater distinguished lecture series, and the Zerner Graduate Fellowship Award. It is easy to make your tax-deductible gift through the University of Florida Foundation. Please make checks out to the University of Florida Foundation and write in the "memo line" which initiative you wish to support: "QTP-Sanibel," "QTP-Löwdin," or "QTP-Zerner." Mail checks c/o Ms. Judy Parker, Quantum Theory Project, University of Florida, PO Box 118435, Gainesville FL 32611-8435. Your continued support is deeply appreciated.

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