

Computational Chemistry and Molecular Modeling Solutions for Chemical and Materials Industry

30.10.2008

The Trinity Centre

24 Cambridge Science Park

Milton Road

Cambridge CB4 0FN

United Kingdom

<http://www.thetrinitycentre.com>

About FUJITSU Seminar

The forthcoming seminar in Cambridge is the first of our planned series of seminars dedicated to computational chemistry. We would like to draw the attention of commercial research and development centers to the latest scientific software solutions for chemical and materials industry. To achieve this goal we decided to prepare a seminar that covers general aspects of use of computational chemistry and molecular modeling in the mentioned industries, with special focus on specific applications in different fields such as microelectronics, glass research and toxicity.

On the other hand, our two most recently released products – Materials Explorer 5.0 and SCIGRESS v.1, represent the highest quality scientific software introducing some of the most recent solutions in the subject. The highest level of expertise of Fujitsu software engineers, as well as some of the most recent algorithms and solutions available, make our software one of the most competitive and advanced solutions for industrial partners.

All of our speakers, including our special guests – Dr. Akira Takada from Asahi Glass Co. Ltd, Dr. Chioko Kaneta from Fujitsu Laboratories Japan and Dr. Stan van Gisbergen from Scientific Computing & Modelling (SCM), represent the top level of expertise in the fields of molecular modeling and computational chemistry. They have many years of professional experience both with the development and application of scientific software in the cutting-edge research work.

We hope that our seminar will attract your attention.

FUJITSU Computer Chemistry Systems - Profile

The Computer Chemistry Systems (CCS) Group of Fujitsu draws upon the rich pipeline of the Fujitsu internal development laboratories and strategic technology partnerships to offer integrated hardware and software solutions designed to enable experimental scientists to bridge the gap between in silico prediction and experimental validation.

Using both proven methodologies and novel approaches, these solutions support the visualization of molecular phenomena, hypothesis development, and experimental validation in chemical research, pharmaceutical design, biotechnology, drug development and materials science research.

- **Integrated in silico prediction and experimental validation tools from a world technology leader**
- **Over 20 years of experience dealing with hardware and software solutions in biosciences and materials science markets**
- **Backed by the resources and commitment of a \$45 billion world technology leader**

The Fujitsu Computer Chemistry Systems Group has its development activities in Krakow (Poland), Beaverton (Oregon, USA), and in Japan. Group members have years of experience in a wide range of fields including polymer and synthetic chemistry, dyes, molecular biology, pharmaceutical discovery, materials science, and computational and experimental methods. Combining practical experience with the deep resources of a world technology leader, the Fujitsu Computer Chemistry Systems Group is prepared to be your partner in applying established techniques and promising new technologies to today's challenges.

As a provider of cutting-edge technology Fujitsu faces challenges rooted in fundamental materials science research, from design of polymers and ceramic materials, to nano-materials. Materials Explorer™ compliments Scigress Explorer™ allowing scientists involved in materials science and chemical research access to simulation and analysis methods through an easy to use desktop application. Our software has been used to study a wide range of systems including, III-V compound semi-conductors, quantum dots, oxide ceramics, and antiferroelectric liquid crystals.

FUJITSU Corporate Profile

Fujitsu is a leading provider of IT-based business solutions for the global marketplace. With approximately 160,000 employees supporting customers in 70 countries, Fujitsu combines a worldwide corps of systems and services experts with highly reliable computing and communications products and advanced microelectronics to deliver added value to customers. Headquartered in Tokyo, Fujitsu Limited (TSE:6702) reported consolidated revenues of 5.3 trillion yen (US\$53 billion) for the fiscal year ended March 31, 2008.

Did You Know?

- Fujitsu is the world's third-largest IT services provider and Japan's market leader.
- Fujitsu and Fujitsu Siemens Computers together are among the world's top five providers of servers.
- Fujitsu customers include nearly half the Fortune Global 500.
- Fujitsu innovations have garnered over 34,000 patents.
- Included in the Dow Jones Sustainability Indexes and FTSE4Good Index Series, Fujitsu is recognized as an IT industry leader in sustainability and corporate responsibility.

Fujitsu at a Glance:

Corporate Headquarters: Fujitsu Limited
Shiodome City Center
1-5-2 Higashi-Shimbashi
Minato-ku, Tokyo 105-7123, Japan

Established: June 1935

President: Kuniaki Nozoe

Business Segments: **Technology Solutions**
System Platforms

- System Products
- Network Products

 Services

- Solutions / Systems Integration
- Infrastructure Services
- Others

Ubiquitous Product Solutions

- PCs / Mobile Phones
- Hard Disk Drives
- Others

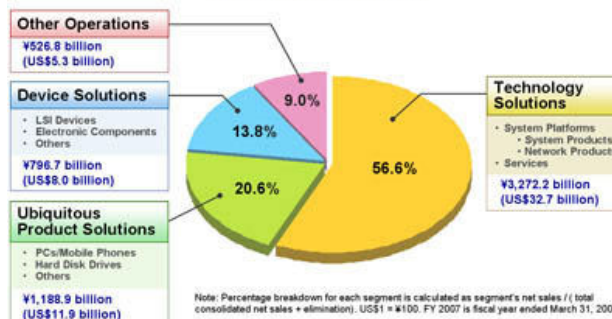
Device Solutions

- LSI Devices
- Electronic Components, Others

Employees: 167,000 (Fujitsu Group worldwide as of March 2008)

Revenue* : 5,330.8 billion yen

FY2007 Consolidated Net Sales by Business Segment, Including Intersegment Sales



Net Income*: 48.1 billion yen

R&D Expenditure*: 258.7 billion yen

Stock Information: Fujitsu Limited shares are listed on the Tokyo Stock Exchange (Code: 6702), as well as the Osaka, Nagoya, Frankfurt, London and Swiss exchanges.

Seminar Schedule

10:00 – 10:20

"Introduction"

Anna Kuzak
FUJITSU

10:20 – 11:20

"Applications of Computational Chemistry and Future Directions for Innovative Solutions in Industry"

Dr. Akira Takada
ASAHI GLASS CO. Ltd.
Visiting Professor of the University College London

11:20 – 11:45

Coffee Break

11:45 – 12:30

"Modern Computational Solutions for Chemical and Materials Industry"

Wojciech Plonka
FUJITSU

12:30 – 13:30

Lunch Break

13:30 – 14:30

"Thermal properties of Gate Dielectrics for Advanced Silicon Devices"

Dr. Chioko Kaneta
FUJITSU LABORATORIES JAPAN

14:30 – 15:30

"The ADF2008 release: new developments and applications in DFT"

Dr. Stan van Gisbergen
SCIENTIFIC COMPUTING & MODELLING (SCM)

15:30 – 16:30

"Use of SCIGRESS and Materials Explorer Software"

Wojciech Plonka/Mateusz Galuszka
FUJITSU

16:30 – 16:45

Coffee break

16:45 – 17:30

"Application of QSAR/QSPR methodology for the study of toxicity of chemical substances"

Wojciech Plonka
FUJITSU

Invited Speakers Profiles

Dr. AKIRA TAKADA

AFFILIATION (1):

Research Center, Asahi Glass Co., Ltd.,
1150 Hazawa-cho, Kanagawa-ku,
Yokohama 221-8755, Japan

AFFILIATION (2):

Department of Chemistry
University College London
Gower Street, London W1E6BT, UK
Visiting Professor

EDUCATION

Tokyo University, Japan, 1973-1977
Bachelor of Engineering; Instrumental Physics and Mathematical Engineering
University College London, 1992-1994
M. Phil & PhD, Geological Sciences

PRESENT ACADEMIC AND GOVERNMENTAL ACTIVITIES

- 2004 to present Visiting professor at chemistry department and Earth Sciences department of University College London (UK) 2002 to 2007 Visiting lecturer at the University of Kyoto (Japan)
- 1996 to present Member of steering committee of division of chemical information and computer science, the Chemical Society of Japan
- 2005 to present Member of steering committee of next-generation super computer national project
- 2007 to present Chairperson of operational committee at Industrial Committee for Supercomputing Promotion

PRESENT INDUSTRIAL COMMUNITY ACTIVITIES

- 2002 to present Chairperson of steering committee of computer chemistry division of ASPRONC (The Association for the Progress of New Chemistry)
- 2005 to present Chairperson of steering committee of Industrial committee for super computing promotion

RESEARCH FIELDS

- Computational Chemistry, Computational Physics, Glass Science, Nano Simulation

RECENT SELECTED PUBLICATIONS

- A. Takada, A.N. Cormack, "Computer simulation models of glass structure", Physics and Chemistry of Glasses: European Journal of Glass Science and Technology, B49, 127-135 (2008).
- A. Takada, "Molecular Dynamics Simulation of deformation in SiO₂ and Na₂O-SiO₂ glasses", Journal of the Ceramic Society of Japan, 116, 880-884 (2008).
- A. Takada, P. Richet, C.R.A. Catlow, G.D. Price, "Molecular dynamics simulation of temperature-induced structural changes in cristobalite, coesite and amorphous silica", J. Non-Cryst. Solids, 354, 181-187 (2008).
- G. Ferlat, T. Charpentier, A.P. Seitsonen, A. Takada, M. Lazzeri, L. Cormier, G. Calas, F. Mauri, Phy. Rev. Lett., 101, 065504 (2008).
- A. Takada, P. Richet, C.R.A. Catlow, G.D. Price, "A molecular dynamics simulation of structural changes in amorphous silica at high temperatures", Eur. J. Glass Sci. Technol., B48, 182-187 (2007).
- A. Takada, P. Richet, C.R.A. Catlow, G.D. Price, "Molecular dynamics simulation of polymorphic and polyamorphic transitions in tetrahedral network glasses: BeF₂ and GeO₂", J. Non-Cryst. Solids, 353, 1892-1898 (2007).

Invited Speakers Profiles

Dr. CHIOKO KANETA

AFFILIATION:

Fujitsu Laboratories, Ltd.
10-1 Morinosato-Wakamiya
Atsugi 243-0197
Japan

EDUCATION

Tohoku University, Sendai, Japan, 1980, 1982, 1985
BS, MS and PhD, Physics

PRESENT ACADEMIC AND GOVERNMENTAL ACTIVITIES

- 2004 to present Specially Appointed Professor of Osaka University
- Member of the Japan Society of Applied Physics

RESEARCH FIELDS

- Molecular Simulations, Computational Physics, Semiconductor Materials

RECENT SELECTED PUBLICATIONS

- C. Kaneta, T. Yamasaki, "Oxygen-related defects in amorphous HfO₂ gate dielectrics", *Microelectronic Engineering*, 84 (9-10), 2370-2373, 2007
- N. Takahashi, T. Yamasaki, and C. Kaneta, "Molecular Dynamics Study of Oxidation Process with SiO emission in the Si/SiO₂ Interface", *ISCSI (International Symposium on Control of Semiconductor Interfaces)*, 2007
- Y. Kosaka, T. Yamasaki, and C. Kaneta, "Molecular Dynamics Simulation on the Crystallization of HfO₂, Hf-aluminate, and Hf-silicate", *Extended Abstracts of the 2003 International Conference on Solid State Devices and Materials, Tokyo*, 822-823, 2003
- T. Yamasaki, C. Kaneta, T. Uchiyama, T. Uda, and K. Terakura, "Geometric and electronic structures of SiO₂/Si(001) interfaces", *Phys.Rev. B*, 63, 115314 (2001)

Invited Speakers Profiles

Dr. STAN VAN GISBERGEN

AFFILIATION:

Scientific Computing & Modelling NV
Vrije Universiteit, Theoretical Chemistry
De Boelelaan 1083
1081 HV Amsterdam
The Netherlands

BIOGRAPHY:

After studying theoretical solid-state physics, Dr. van Gisbergen started in 1994 as a Ph.D. student in the Theoretical Chemistry group of Prof. Baerends at the Vrije Universiteit in Amsterdam.

Dr. van Gisbergen obtained the Ph.D. degree for work on theory development of Time-Dependent DFT and its implementation in the Amsterdam Density Functional (ADF) program. He was awarded the 1998 DSM award for the best thesis in Chemistry and Chemical Technology in The Netherlands in that year.

Dr. van Gisbergen stayed in Prof. Baerends' group as a postdoc working on linear scaling and parallelization of the ADF code from 1998-2000. Then he joined the company Scientific Computing & Modelling in 2000, and he has been leading the company since 2001.

ABOUT ADF:

ADF: the universal density functional package for chemists

The Amsterdam Density Functional (ADF) package is software for first-principles electronic structure calculations. ADF is used by academic and industrial researchers in such diverse fields as pharmacochemistry and materials science. It is particularly popular in the research areas of homogeneous and heterogeneous catalysis, inorganic chemistry, heavy element chemistry, various types of spectroscopy, and biochemistry.

Registration Form

The participation in FUJITSU seminar is free of charge. Please fill all the fields below:

Name

Surname

Title

Company/Institution Name

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Company/Institution Address

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E-mail address

Phone Number

Fax

In order to register for the FUJITSU Seminar, please send the registration form by e-mail (address: ccs@fqs.pl) or fax (fax number: +48 12 429 61 24).

The deadline is 14.10.2008.

In case of any questions, please contact:

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FUJITSU

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