

One day conference on Quantumwise Nanoscale device simulation package At CDAC Noida, Sector 62, Noida (UP) On March 26th 2009

School of Electronics, CDAC, Noida and Integrated Microsystems jointly announce a one day workshop on **Quantumwise Nanotechnology package**. The workshop aims at introducing and advance training to researchers/engineers to modeling of nanoscale devices.

Talk Abstract

Using Ab initio and semi-empirical modelling to assist both theoreticians and experimentalist in predicting and understanding the behavior of nanoscale devices.

As the dimensions of electronic devices are rapidly decreasing, there is a need for a new generation of modeling tools that can accurately calculate the electrical properties of devices where atomic scale details and quantum effects are important.

A promising framework for such calculations is density functional theory within the non-equilibrium Green's function formalism (NEGF-DFT) [1,2]. In addition, for the formalism to be applied in semiconductor device modeling it needs to be able to handle many thousands of atoms. We discuss new developments and future aspects [3,4] of the method important for semiconductor device modeling; in particular we show that for important classes of systems the approach scales linearly with the system size.

First-principles simulation software for nanoscience:

QuantumWise software is used to model the electronic structure of molecules, crystals, and surfaces. It is distinguished by its unique capability to simulate electrical transport in nano-devices, and its ability to treat large-scale systems. The QuantumWise platform is based on an open architecture which integrates a powerful scripting language with a GUI platform. The software is actively used in a wide range of application areas such as:

- **Molecular electronics**
- **Carbon nanotubes and graphene**
- **Nanowires**
- **Computational material science**
- **Bulk and nanoscale semiconductors**
- **Surface electrochemistry**
- **Magnetic systems**

The QuantumWise platform, based on an open architecture which integrates a powerful scripting language with a GUI platform consists of a core component called Atomistix ToolKit (ATK) and a user-friendly graphical interface called Virtual NanoLab. It provides simple and intuitive access to state-of-the-art atomic advanced modeling techniques such as non-equilibrium Green's functions (NEGF) and density functional theory (DFT) thus allowing the user to focus on the physical properties of the systems under investigation instead. For more information, kindly refer to www.quantumwise.com

Expected Participants : Scientists/Professors/Faculty members/Engineers, currently teaching and likely to teach courses related to VLSI design/Process/Device simulation.

Registration : Limited to 35 Participants (selected on First come first server basis). You can register by sending an email to info@ims-india.org or artinoor@cdacnoida.in on or before 25th March,2009.

INTEGRATED MICROSYSTEM

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1 DAY NANO WORKSHOP USING QUANTUMWISE NANOLAB By Dr.Kurt Stokbro (CEO, Quantumwise)

At Venue is B-30, Auditorium, Academic block, Sector -62, CDAC Noida

Conference Agenda

26th March, 2009

9:45 a.m	- 10.00a.m	Company Introduction
10.00a.m	- 11.30a.m:	Using Ab initio and semi-empirical modelling to predict and understand the behavior of nanoscale devices.
11.30a.m	-11.45a.m:	Tea Break
11.45a.m	- 01.30p.m:	Introduction to Quantumwise Tools: Atomistix Toolkit (ATK) and Virtual Nanolab (VNL)
1.30p.m	- 2.30p.m:	Lunch Break
2.30p.m	-5.00p.m:	Live demonstration on Virtual Nanolab and ATK Session (Covering examples like Carbon nanotubes, Nanowires, Magnetic tunnel, nanoribbons, spintronic devices etc.)
5.00p.m	-5.15p.m	Discussion

About the Speaker

Dr. Kurt Stokbro

- Entrepreneur and researcher with focus on atomic-scale simulations;
- Co-founder and CEO of Atomistix Aps, Atomistix Inc., QuantumWise A/S
- Organizer of research projects with total USD 5 million in funding;
- Large network of researchers in academia and industry in Europe, USA and Asia.
- Formerly a Professor with the Copenhagen University, Denmark;
- Recognized researcher with 58 publications in refereed journals, >1500 citations and 28 invited talks at international conferences.
- Member of the scientific advisory board of IRC in Nanotechnology (University of Cambridge, University College London and the University of Bristol) and the scientific advisory board of Center for Atomic-scale Materials Design (CAMD), Technical University of Denmark.
- Participation in the modeling section of the International Technology Roadmap for Semiconductors (ITRS);
- Organizer of 3 international conferences within atomic-scale simulations;