

**Agenda for
ATOMCAD Meeting
Paris, Dec. 13th, 2002
Hotel Claude Bernard, rue des Ecoles**

9h - 9h05	Introduction by the Project Officer
9h05 – 10h	Coordinator Report and discussion on Scientific, Networking, Training and Administrative aspects
10h – 10h30	Coffee Break
10h30 – 12h	Tour de Table by Participating Teams and discussion
12h – 14h	Lunch
14h – 15h	Meeting between Young Researchers and the Project Officer
15h – 16h	Young Researcher's Report
16h – 16h15	Coffee Break
16h15 – 16h45	Meeting between coordinator, the scientists in charge and the project officer
16h45 – 18h	Open Discussion and Recommendations
18h	End of the Meeting

Participants : Bruno Schmitz (Head of RTN Unit), Gordana Popovic (ATOMCAD Project Officer), Servane Blanque (CNM), Mehdi Djafari Rouhani (LAAS/LPST), Alain Estève (LAAS), Jim Greer (NMRC), Léonard Jeloica (LAAS), Andreas Larsson (NMRC), Bengt Lundqvist (Chalmers Univ.), Philippe Paillet (CEA), Jose Rebollo (CNM), Nicolas Richard (CEA), Riccardo Rurali (CNM), Elwira Wachowicz (Chalmers Univ.),

The review meeting of ATOMCAD network was held in Paris on Dec. 13th 2002. The EU officers in charge of RTN programme were present at this meeting

1 - Partner presentation

The meeting started by the presentation of ATOMCAD partner institutions and activities, present at the meeting.

NMRC : Computational modelling group

Staff : 6 permanents, 2 post docs + 2 vacant positions, 8 PhD + 3 vacant positions

Main interests :

- Continuum modelling,
- Thermo-mechanical modelling,
- Physical device Modelling,
- Microsystems,
- Si/SiO₂ and oxides,
- Molecular electronics

CNM

CNM is one of three centres of CSIC (Spanish national research organisation). The centres are in Madrid, Barcelona and Sevilla

Main interests :

- SiC oxidation
- SiC doping by implantation and annealing

LAAS/LPST : Modelling Team

Staff : 6 permanents, 1 post docs vacant position, 3 PhD

Main interests :

- Oxidation of silicon,
- High -k material deposition
- Molecular grafting on silicon for biological applications,
- Heteroepitaxial growth of semiconductors,
- Dynamics of disordered systems,
- Molecule - molecule interaction for DNA - Protein Docking

CEA

Main interests :

- Hardening against radiation,
- Electrical behaviour of irradiated devices,
- Reliability of devices,
- Process modelling (TRAPPOX software package).

Chalmers Univ. of Technology: Surface Theory Group

Staff : 25 permanents, 13 PhD

Main interests :

- C in graphite,
- Long range interaction (Van der Waals) using LDA and GGA approximations

2 - Young Researchers

The following Young researchers have been recruited :

- Andreas LARSSON at NMRC as post-doc, to work on quantum chemistry study of dopant states in semiconductors and fullerenes,
- Riccardo RURALI at CNM as a pre-doc, to work on the modelling of SiC processing (diffusion, oxidation) for SiC based electronic devices,
- Otilia BISERICA at CNM as pre-doc, to work on the technological processing of SiC,

- Sevane BLANQUE at CNM as a pre-doc, to continue the work of Otilia BISERICA on SiC processing after she left CNM,
- Leonard JELOAICA at LAAS as a pre-doc, to work on molecule-surface interaction for application to Atomic Layer Deposition of high -k material and for biological applications,
- Elwira WACHOWICZ at CUT as a post doc, to work on DFT calculations related to SiC and ZnO materials

vacant positions

- 1 post-doc at LAAS,
- 1 post-doc at SIGMAPLUS,
- 1 post-doc at CEA.

3 - Conclusion

The details of scientific work presented here are reported in the mid-term review report.

It has been stated, at this meeting, that there has been some overlooking regarding the administration : reporting, management. However, the discussion of EU officers with Young Researchers has proved successful in the sense that they are all involved in scientific topics of current international interest and that they feel progressing in their perspective of training by research.

The future meeting of ATOMCAD is programmed for February 2003 where we should discuss some reorientation of the project for the last period of the network in order to fulfil its primary goals.