
**Research Networking Programmes**

# Science Meeting – Scientific Report

***Proposal Title:***

12th ETSF Young Researchers' Meeting:
Challenges in *ab initio* Modelling of Materials and Molecules

***Application Reference N°:*** 5766

## 1. Summary

The 12th ETSF Young Researchers' Meeting (YRM) entitled "Challenges in *ab initio* Modelling of Materials and Molecules" took place on the Jussieu campus of the Université Pierre et Marie Curie in Paris (France) from 1 to 5 June 2015. The ETSF (European Theoretical Spectroscopy Facility) is a European network that unites the expertise of more than 200 researchers in the field of *ab initio* theoretical spectroscopy for solids and molecular systems. The Young Researchers' Meeting gives non-permanent researchers from within and outside the network the chance to present and discuss their scientific research projects. In total, the meeting has been attended by 65 young researchers (master students, PhD students, and postdocs).
The meeting addressed problems and recent achievements in method development (density-functional theory, Green's function theory, ...), algorithms and implementations, as well as applications to materials. The 12th edition of the YRM focused mainly on the following topics:

- crystal-structure prediction,
- thermal transport,
- electronic, magnetic, and optical properties,
- strongly correlated phenomena,
- ultrafast dynamics.

At the beginning of each session, experienced postdocs gave keynote talks to provide the participants with an overview of the field, an explanation of the theoretical

framework of the relevant physical problems, and a review of the state-of-the-art computational methods. A large number of attendees presented their research project in contributed talks. Moreover, a poster session was organized. Almost all participants took the chance to present their work at the meeting (talk or poster).
An entire day was dedicated to research in an industrial context giving the participants the opportunity to discover research outside academia. It included invited talks by theoretical physicists working in industry, a round-table discussion with the audience, and a job market during the poster session.
Various social activities which took place in the evening fostered the friendly atmosphere that prevailed at the meeting. The scientific discussion, which was intense but constructive, benefitted from this ambiance of mutual trust.

## 2. Description of the scientific content and discussions at the event

### Crystal-structure prediction

Zamaan Raza gave the introductory talk on the problems of crystal-structure prediction. He addressed the question of the stability of a given atomic configuration which can be answered efficiently by total-energy calculations using density-functional theory (DFT). Second, he discussed search algorithms to identify potentially stable configurations in the high-dimensional space of possible configurations. The success of these methods was illustrated by examples from planetary science, superconductivity, and materials design.
The contributed talks of this session discussed new methods to predict the structure of nanomaterials (bimetallic alloy nanoparticles, ceria with oxygen vacancies), the self-assembly of organic molecules on insulating surfaces, and materials design using perovskite oxide superlattices with orbital ordering. Moreover, a study on cerium-doped lanthanum silicon nitride phosphors for white LEDs has been presented.

### Thermal transport

The keynote talk was given by Claudio Melis. He spoke about thermal transport at the nanoscale in the context of nanoelectronics, photovoltaics, and thermoelectric devices. Recent progress in theoretical and computational methods for calculating thermal conductance and phonon scattering was reported. A particular emphasis was given to the approach-to-equilibrium molecular dynamics technique.
In this session, equilibrium and non-equilibrium molecular dynamics simulations for the thermal conductivity of silicon nanowires, calculations of the thermal properties of bismuth using the Boltzmann transport equation, and an *ab initio* description of the phonon-drag effect in semiconductors were shown.

### Electronic, optical, and magnetic properties

Maria Hellgren introduced the field of electronic, optical, and magnetic excitations in solids. She focused on the derivation of widely used methods in many-body theory (Hartree-Fock, *GW*, Bethe-Salpeter equation) by means of variational approaches.

Moreover, the Green's function approaches were compared to DFT and its time-dependent extension (TDDFT). She also talked about the application of the many-body techniques to new exotic phases of matter such as charge-density waves in 2D layered systems.
In this session, a reformulation of Hedin's equations using a path-integral formalism has been presented. Speakers reported on DFT calculations with hybrid functionals for the electronic structure of metal-doped semiconductors (which may serve as absorbers for intermediate-band solar cells) and the performance of hybrid functionals with parameters obtained from many-body perturbation theory. Research projects were presented where TDDFT has been used to calculate the electronic stopping power in silicon carbide, excited-state spectra of polyacenes for room-temperature masers, or fluorescence spectra in amyloid proteines. Moreover, a linearly scaling TDDFT implementation for low-energy excitations in systems with thousands of atoms has been demonstrated.
Talks have been given on finite-temperature potential functional theory for describing matter at extremely high pressures and temperatures, plasmonic field enhancement in nanostructures, high-harmonic generation in hydrogen atoms using time-dependent configuration interaction, and local-field effects in surface second-harmonic generation. Spin-polarized very-low-energy electron diffraction calculations of an oxygen-passivated iron surface for a spin filter which exploits exchange and spin-orbit scattering have been presented. Moreover, the progress in the development of an *ab initio* approach for describing x-ray magnetic circular dichroism, a technique which allows to access spin and orbital contributions to magnetic moments, has been sketched.

**Strongly-correlated phenomena**

Priyanka Seth introduced the concept of strongly correlated systems. She bridged the gap between model systems (e.g. Hubbard model) and real solids. A strong focus of her presentation was on the virtues of seemingly simple models that allow one to understand the physics of a correlated system qualitatively.
In this session, an advanced dynamical mean-field theory (DMFT) framework to describe the physics of self-assembled rare-earth superlattices on metallic surfaces, which can be used for magnetic data storage, has been presented. A strong focus of the session lied on the combination of DMFT with *GW* and the difficulties of such an approach. Moreover, reduced density-matrix functional theory for the calculation of the one-body spectral function and the strictly-correlated-electrons limit of DFT to obtain molecular dissociation energies were discussed. Calculations of the superconducting transition temperature of alkali-doped fullerides using DMFT and a downfolding scheme for the electron-phonon coupling were shown. The last part of the session was dedicated to Kondo physics: The description of the Kondo effect using a multi-orbital Anderson impurity model as well as the simulation of its experimental manifestation as Fano resonances in scanning tunnel spectroscopy of magnetic adatoms on metallic surfaces have been illustrated.

**Ultrafast dynamics**

Davide Sangalli gave the keynote talk on ultrafast dynamics. He introduced real-time TDDFT and compared to frequency-space approaches. Moreover, he focused on out-of-equilibrium systems and sketched their description on the Keldysh contour.

The contributed talks of this session dealt with charge and spin dynamics in solids beyond the linear-response regime, the construction of a new functional for (TD)DFT guided by insight from the time propagation of the exact many-electron wave function in correlated 1D systems, and the semi-empirical density-functional tight-binding theory to describe charge-transfer processes in the attosecond regime. Moreover, works on strong-field effects in photoemission and real-time electron dynamics in quantum systems that are coupled to a dielectric medium were presented.

**Industry day**

One of the main objectives of the YRM was to increase the awareness of the participants for career perspectives in research outside academia. To this end, the first day of the meeting was dedicated to research in an industrial context:

- Julien Vidal, representing EDF and the Institut Photovoltaïque d'Île-de-France (IPVF), talked about *ab initio* simulations of photovoltaic absorbers (stability issues, defect formation, band-gap engineering).

- Lorenzo De Leo, representing Capital Fund Management, gave an introduction into finance and showed mathematical models to calculate the value of options on stock markets.

- Hartmut Hafermann, representing Huawei Technologies, gave an overview on the use of Monte-Carlo simulations in information technology and the development of the next-generation mobile communication standards.

All speakers of this session had obtained a PhD in theoretical solid-state physics and had gained research experience as postdoc before they moved to the private sector. In their talks, they presented, apart from their present research topics, the motives for their decision to pursue their career in the private sector as well as the advantages and drawbacks of working in academia or industry.
In the afternoon, the participants of the YRM had the occasion to ask questions about research in industry during a moderated round-table discussion with the speakers from the morning session. The discussion was so lively that the session had to be extended and took 90 instead of the planned 60 min. The questions touched, among others, upon industrial secret, hierarchy, profit-oriented research, long-term vs. short-term projects, freedom of research, salaries, and work-life balance.
The discussion continued during the poster session where the industry representatives were also present. The IPVF presented job offers for PhD and postdoc positions at the job market which was integrated in the poster session.

**Gender issues**

Anne Pépin from the CNRS gave a presentation about conscious and subconscious gender discrimination in science, and in particular in physics. Even though the presentation focused on the French system, she gave interesting examples of sociological experiments proving the existence of prejudices with respect to women in science in various societies. Her talk triggered a lively discussion on gender discrimination.

## 3. Assessment of the results and impact of the event on the future directions of the field

The number of registered participants exceeded the organizers' expectations. In order to allow all applicants to participate, the meeting had to be moved to a bigger lecture hall. The attractiveness of the meeting to young researchers in the community is further illustrated by the large number of applications from outside the ETSF. The mixture of ETSF and non-ETSF participants ensured a scientific exchange that reaches beyond the limits of the ETSF network.

The number of requests for oral presentations was significantly bigger than the number of available slots. A selection has been made upon the submitted abstracts taking into account the scientific experience of the participant to avoid discrimination of young researchers in the earliest stages of their career. This procedure ensured that also participants in the first years of their PhD studies got the chance to present their work to an international audience, train their communication skills, and receive feedback from their peers. The balance between different experience levels is illustrated by the repartition of contributed talks: 22 % PhD students (first 2 years), 37 % PhD students (more than 2 years), 25 % postdocs (first 2 years), 16 % postdocs (more than 2 years).

From the organizers' point of view, the meeting has been very successful. The keynote speakers who gave pedagogical introductions to the five sessions of the meeting all succeeded in bridging the gap between the fundamental concepts of their field, the utilized numerical techniques, and the practical applications. This allowed participants whose own research project is situated in one of the other fields to follow all the talks of each session.

The quality of the contributed talks was exceptionally high. The contributed speakers managed to give comprehensible talks on their research topics, explaining the physics that is behind and not merely the technical details of their calculations. A strong focus of the meeting lied on creating an atmosphere of mutual trust in order to stimulate scientific discussion. This objective has been fully attained. Almost all talks incited a lively discussion and a high number of questions by the young researchers in the audience. Also the poster session was a clear success. The discussion of the presented research projects was so intense that the finger food served during the poster session was almost abandoned.

The participants of the meeting received valuable criticism by their peers which will allow them to explore yet non-elucidated aspects of their research projects. Some young researchers could also benefit from the experience of the others with the technical aspects of their work (e.g. which code to use, aspects of convergence and parallelization, ...). By following the talks from different sessions, the attendees of the meeting could broaden their knowledge on the methods, approaches, and techniques used in the field of theoretical spectroscopy for solids and molecular systems.

The industry day was very much appreciated by the participants. In particular, they valued the fact that the speakers did not only present the achievements of their companies, but gave an honest overview on a researcher's life in industry. This insight may have a strong impact on the future career decisions of the young researchers.

In the evening, various social activities were organized in order to foster a friendly atmosphere and allow the participants to create personal links with their peers. On Tuesday night, the traditional improvised "YRM football match" took place in the Parc de Bercy.

On Thursday night, the participants could take part in a walking tour around the most famous historical sights of Paris before the social dinner. The social dinner at the Café du Commerce was highly appreciated by the attendees of the meeting. In the evenings without organized program, the participants gathered spontaneously, e.g. for a picnic at the bank of the Seine. Hosting the attendees of the meeting in the same hostel contributed to improving the sense of community.
The organizers received very positive feedback from the participants about the organization of the meeting and the scientific program. Young researchers from King's College London volunteered for organizing the next ETSF Young Researchers' Meeting in London (United Kingdom) in 2016.

# Annex 4a: Programme of the meeting

| Time | 1 June Monday |
|---|---|
| 09:00 | Registration |
| 09:30 | EDF / IPVF |
| 10:15 | *Coffee* |
| 10:40 | CFM |
| 11:25 | Huawei |
| 12:10 | *Lunch* |
| 14:10 | Round Table |
| 15:10 | *Break* |
| 15:30 | Poster Session<br>Job Market |

| Time | 2 June Tuesday |
|---|---|
| 09:00 | Raza |
| 09:50 | Kozlov |
| 10:15 | Paris |
| 10:40 | *Coffee* |
| 11:05 | Kocak |
| 11:30 | Jia |
| 11:55 | Coccia |
| 12:20 | *Lunch* |
| 14:20 | Hellgren |
| 15:10 | Gerosa |
| 15:35 | Tancogne |
| 16:00 | *Coffee* |
| 16:25 | Shukri |
| 16:50 | Grisanti |
| 17:15 | Vanzini |
| | Sports |

| Time | 3 June Wednesday |
|---|---|
| 09:00 | Sangalli |
| 09:50 | Elliott |
| 10:15 | Hodgson |
| 10:40 | *Coffee* |
| 11:05 | Boleininger |
| 11:30 | Gao |
| 11:55 | Pipolo |
| 12:20 | *Lunch* |
| 14:20 | Gender Issues |
| 15:10 | McMillan |
| 15:35 | Zuehlsdorff |
| 16:00 | *Coffee* |
| 16:25 | Cangi |
| 16:50 | Borek |
| 17:15 | Mas |

| Time | 4 June Thursday |
|---|---|
| 09:00 | Seth |
| 09:50 | Blackbourn |
| 10:15 | Pisanti |
| 10:40 | *Coffee* |
| 11:05 | Di Sabatino |
| 11:30 | Vuckovic |
| 11:55 | Nomura |
| 12:20 | *Lunch* |
| 14:20 | Melis |
| 15:10 | Xiong |
| 15:35 | *Coffee* |
| 16:00 | Markov |
| 16:25 | Kane |
| | Excursion |
| | Dinner |

| Time | 5 June Friday |
|---|---|
| 09:00 | |
| 09:50 | Motahari |
| 10:15 | Frank |
| 10:40 | *Coffee* |
| 11:05 | Bogatko |
| 11:30 | Koskelo |
| 11:55 | Farewell |

| | | |
|---|---|---|
| Industry | Thermal transport | Strongly corr. phenomena |
| Crystal-structure pred. | Elec., magn., opt. prop. | Ultrafast phenomena |

## Monday, 1 June 2015 – Industry day

| | |
|---|---|
| 09:00 – 09:30 | Registration and opening speech |
| 09:30 – 10:15 | Julien Vidal – EDF and IPVF<br>*First principles calculations in an industrial context: The case of photovoltaic technologies* |
| 10:15 – 10:40 | Coffee break |
| 10:40 – 11:25 | Lorenzo De Leo – Capital Fund Management<br>*Trading options electronically* |
| 11:25 – 12:10 | Hartmut Hafermann – Huawei Technologies<br>*Research in industry – leveraging a theoretical physics background in telecommunications* |
| 12:10 – 14:10 | Lunch |
| 14:10 – 15:10 | Industry round table |
| 15:10 – 15:30 | Break |
| 15:30 – 18:00 | Poster session with job market |

**Tuesday, 2 June 2015**

| | |
|---|---|
| 09:00 – 09:50 | Zamaan Raza – Keynote talk<br>*An introduction to crystal structure prediction* |
| 09:50 – 10:15 | Sergey M. Kozlov<br>*Novel Methods for Structure Prediction in Nanomaterials* |
| 10:15 – 10:40 | Chiara Paris<br>*Surface phase transition driven by deprotonation reaction* |
| 10:40 – 11:05 | Coffee break |
| 11:05 – 11:30 | Aysegul Begum Kocak<br>*First Principle Study of Oxide Superlattices* |
| 11:30 – 11:55 | Yongchao Jia<br>*Ab-initio study of lanthanum silicon nitride phosphor for white LEDs* |
| 11:55 – 12:20 | Emanuele Coccia<br>*High harmonic generation spectrum of the hydrogen atom using time-dependent configuration interaction: results from length and velocity gauge* |
| 12:20 – 14:20 | Lunch |
| 14:20 – 15:10 | Maria Hellgren – Keynote talk<br>*Correlation effects in molecules and solids from a variational formulation of many-body perturbation theory* |
| 15:10 – 15:35 | Matteo Gerosa<br>*Electronic structure and total energies of oxide semiconductors with many-body perturbation theory based hybrid functionals* |
| 15:35 – 16:00 | Nicolas Tancogne-Dejean<br>*Ab initio local field effects for surface second harmonic generation* |
| 16:00 – 16:25 | Coffee break |
| 16:25 – 16:50 | Abdullah A. Shukri<br>*Ab initio calculation of the electronic stopping power* |
| 16:50 – 17:15 | Luca Grisanti<br>*Modeling optical properties in amyloid proteins: proton delocalization and structure-related fluorescence* |
| 17:15 – 17:40 | Marco Vanzini<br>*Hedin Equations and Kohn-Sham Potential in the Path-Integral Formalism* |

**Wednesday, 3 June 2015**

| | |
|---|---|
| 09:00 – 09:50 | Davide Sangalli – Keynote talk<br>*Ultra-fast dynamics* |
| 09:50 – 10:15 | Peter Elliott<br>*Charge and Spin Dynamics in Solids using Real Time TDDFT* |
| 10:15 – 10:40 | Matthew J. P. Hodgson<br>*Electron localisation in exact time-dependent density-functional potentials* |
| 10:40 – 11:05 | Coffee break |
| 11:05 – 11:30 | Max Boleininger<br>*Ultrafast Dynamics in Density-Functional Tight-Binding* |
| 11:30 – 11:55 | Cong-Zhang Gao<br>*Strong-field effects in the photoemission spectrum of the Fullerene* |
| 11:55 – 12:20 | Silvio Pipolo<br>*Quantum electron dynamics in a dielectric medium* |
| 12:20 – 14:20 | Lunch |
| 14:20 – 15:10 | Anne Pépin<br>*Gender issues* |
| 15:10 – 15:35 | Ryan McMillan<br>*Real-Time Modelling of Plasmonic Field Enhancement in Nanostructures* |
| 15:35 – 16:00 | Tim J. Zuehlsdorff<br>*Applications of linear-scaling time-dependent density-functional theory* |
| 16:00 – 16:25 | Coffee break |
| 16:25 – 16:50 | Attila Cangi<br>*Electronic Structure under Extreme Conditions* |
| 16:50 – 17:15 | Stephan Borek<br>*Ab initio calculation of Spin-Polarized Low-Energy Electron Diffraction for the systems Fe(001) and Fe(001)-p(1x1)-O* |
| 17:15 – 17:40 | Nadejda Mas<br>*Ab-initio calculation of K-edge XMCD spectra* |

**Thursday, 4 June 2015**

| | |
|---|---|
| 09:00 – 09:50 | Priyanka Seth – Keynote talk<br>*Strongly-correlated systems: signatures and theoretical approaches* |
| 09:50 – 10:15 | David Blackbourn<br>*DMFT study of self assembled diluted solids composed of strongly correlated d- and f-elements on a substrate* |
| 10:15 – 10:40 | Paolo Pisanti<br>*A new self-consistent QSGW+DMFT description of strongly correlated materials* |
| 10:40 – 11:05 | Coffee break |
| 11:05 – 11:30 | Stefano Di Sabatino<br>*Reduced Density-Matrix Functional Theory: correlation and spectroscopy* |
| 11:30 – 11:55 | Stefan Vuckovic<br>*Dissociating chemical bond in the strictly-correlated regime of density functional theory* |
| 11:55 – 12:20 | Yusuke Nomura<br>*Fully ab initio calculation of superconducting transition temperature for alkali-metal-doped $C_{60}$ solids* |
| 12:20 – 14:20 | Lunch |
| 14:20 – 15:10 | Claudio Melis – Keynote talk<br>*Modeling thermal transport at the nanoscale* |
| 15:10 – 15:35 | Shiyun Xiong<br>*Thermal Transport in Si Nanowires with Periodical pillars* |
| 15:35 – 16:00 | Coffee break |
| 16:00 – 16:25 | Maxim Markov<br>*Thermal properties of bismuth calculated ab initio* |
| 16:25 – 16:50 | Gaston Kané<br>*Phonon drag effect in Silicon: an ab initio approach* |

**Friday, 5 June 2015**

| | |
|---|---|
| 09:50 – 10:15 | Sareh Motahari<br>*Kondo physics of multi-orbital Anderson models studied by distributional exact diagonalization* |
| 10:15 – 10:40 | Sebastian Frank<br>*Orbital signatures of Fano-Kondo lineshapes in STM adatom spectroscopy* |
| 10:40 – 11:05 | Coffee break |
| 11:05 – 11:30 | Stuart Bogatko<br>*Size and Substitution Effects in excited state spectra of polyacenes: application to the room-temperature maser* |
| 11:30 – 11:55 | Jaakko Koskelo<br>*Electronic structure of iron-doped $CuGaS_2$* |
| 11:55 – 12:20 | Farewell |

## Annex 4b: Full list of speakers and participants

### Organizers

Bronstein, Yael, Université Pierre et Marie Curie, France
Chauvin, Sophie, Ecole polytechnique, France
Fugallo, Giorgia, Ecole polytechnique Paris , France
Prussel, Lucie, Ecole polytechnique, France
Reshetnyak, Igor, LSI, Ecole polytechnique, France
Rödl, Claudia, Ecole polytechnique, France
Sponza, Lorenzo, King's College London, United Kingdom
Stan, Adrian, Sorbonne University (alliance), France
Tancogne-Dejean, Nicolas, Ecole polytechnique, France
Tarantino, Walter, Ecole polytechnique, France
Tzavala, Marilena, Ecole polytechnique, France
Zhou, Jianqiang, Ecole polytechnique, France

### Keynote speakers

Hellgren, Maria, Luxembourg University, Luxembourg
Melis, Claudio, Department of Physics - University of Cagliari, Italy
Raza, Zamaan, Linköping University, Sweden
Sangalli, Davide, Istituto di Struttura della Materia (ISM-CNR), Italy
Seth, Priyanka, Ecole Polytechnique, France

### Speakers

Blackbourn, David, King's College London, United Kingdom
Bogatko, Stuart, Imperial College London, United Kingdom
Boleininger, Max, Imperial College London, United Kingdom
Borek, Stephan, LMU Munich, Germany
Cangi, Attila, Max Planck Institute of Microstructure Physics, Germany
Coccia, Emanuele, Laboratoire de Chimie Théorique, UPMC, Paris, France
Di Sabatino, Stefano, Université Paul Sabatier, France
Elliott, Peter, Max Planck Institute of Microstructure Physics, Germany
Frank, Sebastian, Max Planck Institute of Microstructure Physics, Germany
Gao, Cong-Zhang, Université Paul Sabatier, France
Gerosa, Matteo, Politecnico di Milano, Italy
Grisanti, Luca, "Abdus Salam" ICTP, Trieste, Italy
Hodgson, Matthew, University of York, United Kingdom
Jia, Yongchao, IMCN, UCL, Belgium
Kane, Gaston, LSI, Ecole polytechnique, France
Kocak, Aysegul Begum, Institut Neel, France
Koskelo, Jaakko, University of Helsinki, Finland
Kozlov, Sergey, Universitat de Barcelona, Spain
Markov, Maksim, Ecole Polytechnique, France
Mas, Nadejda, IMPMC (UPMC), France
McMillan, Ryan, Queen's University Belfast, United Kingdom

Motahari, Sareh, Max Planck Institute of Microstructure Physics, Germany
Nomura, Yusuke, École polytechnique, France
Paris, Chiara, King's College London, United Kingdom
Pipolo, Silvio, École normale supérieure, France
Pisanti, Paolo, King's College London, United Kingdom
Shukri, Abdullah, SRMP CEA-Saclay, France
Tancogne-Dejean, Nicolas, Ecole polytechnique, France
Vanzini, Marco, LSI, Ecole Polytechnique, France
Vuckovic, Stefan, Vrije University Amsterdam, Netherlands
Xiong, Shiyun, Max Planck Institute for Polymer Research, Germany
Zuehlsdorff, Tim J., University of Cambridge, United Kingdom

**Participants**

Azarhoosh, Pooya, King's College of London, United Kingdom
Chen, Kathy, Université de Nantes, France
Dang, Yiteng, Ecole Normale Superieure, France
Delange, Pascal, Ecole Polytechnique, France
Guzzo, Matteo, Humboldt-Universität zu Berlin, Germany
Khotiaintseva, Tetiana, University Paris XI, France
Li, Dongzhe, Service de Physique de l'Etat Condensé, CEA-Saclay, France
Loach, Christian, University of Edinburgh, United Kingdom
Medvedeva, Daria, Ural Federal University, Ekaterinburg, Russia
Moynihan, Glenn, CRANN Institute, Ireland
Naden Robinson, Victor, The University of Edinburgh, United Kingdom
Pashov, Dimitar, KCL, United Kingdom
Scherrer, Arne, Martin Luther University Halle-Wittenberg, Germany
Teeratchanan, Pattanasak, University of Edinburgh, United Kingdom
Vishina, Alena, King's College London, United Kingdom
Yu, Lantao, EM2C, France
Zakharov, Iaroslav, Ecole Polytechnique, France

**Invited speakers - Industry day**

De Leo, Lorenzo, Capital Fund Management, France
Hafermann, Hartmut, Huawei Technologies, France
Vidal, Julien, EDF R&D, France

**Invited speaker - Gender issues**

Pépin, Anne, CNRS, France