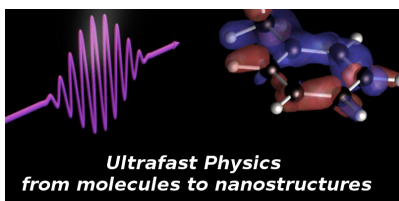


# Ultrafast Physics from molecules to nanostructures



**Proposed dates :**  
*May 20, 2019 - May 24, 2019*  
**Alternative dates :**  
*Sep 02, 2019 - Sep 05, 2019*

**Andrea Marini**  
*National Research Council*

**Gianluca Stefanucci**  
*University of Rome, Tor Vergata, Italy*

**Giulio Cerullo**  
*Polytechnic University of Milan, Italy*

**MAURO NISOLI**  
*Politecnico di Milano*

**Angel Rubio**  
*Max Planck Institute for the Structure and Dynamics of Matter*

**E.K.U. Gross**  
*Max Planck Institute of Microstructure Physics, Halle*

# 1 Proposal

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## 1.1 Short Description of the proposed CECAM/Psi-K conference

The impressive progress in ultrafast laser technology, ranging from the femtosecond to the attosecond timescale and from the THz to the XUV frequency range, is making possible to probe real-time electronic and nuclear dynamics in atoms, molecules and solids[1]. Fundamental insight can be gained into the primary photoinduced processes in systems with growing level of complexity[2]. The capability of following and steering ultrafast dynamics has tremendous impact in a wide range of applications, from materials science[3] to life sciences.

Clearly, advances in theories and methods for modeling ultrafast processes inevitably require an intense exchange with the experimental community due to the complexity of the systems and of the measurements. In the last decade the effort in developing predictive and computationally feasible methods has virtually exploded. Ab initio approaches based on DFT and nonequilibrium Green's function (NEGF)[4] have recently made contact with time-resolved experiments in 2D systems and nanostructures. Other ab initio methods based on wavefunctions (e.g., ADCn, CASPTn) or reduced quantities (e.g., TDDFT, NEGF) for modeling ultrafast processes enable to access the electron-nuclear subfemtosecond dynamics in molecules. Furthermore, accurate real-time numerical methods have been put forward for strongly correlated model systems (e.g., TD-DMFT and DMRG). This workshop will gather world-leading experts in theory and experiments, enabling a cross-fertilization which will enable to advance the state of the art in ab-initio methods. In fact, the rapid development of experimental techniques has not been followed by a simultaneous integration with the ab-initio computational community. The result is a scarce availability of numerical tools for crucial systems of technological or fundamental interest, e.g., biomolecules, large nanostructures and materials with technological application. One of the key challenges is therefore to extend the range of application of material science and chemistry codes to the study of out-of-equilibrium properties. To this purpose, it is crucial to let experimental, theoretical and computational scientists meet and debate on crucial questions like: how to extend the accuracy of ab-Initio methods out-of-equilibrium? How to efficiently benefit from the advances in computation facilities to simulate the nonequilibrium dynamics of complex materials? How to translate laser-pulse features into boundary conditions and suitable approximations for the computational tools? Can we devise a series of tools and procedures to provide to the community?

This workshop aims at being a turning point in ultrafast computational science, settling down crucial and yet unexplored directions to progress. We will compare different theoretical formulations of experimental outcomes, discuss their range of applicability as well as their physical and numerical limitations. We will also discuss for the various approaches how to include the missing physics and whether this inclusion is numerically feasible.

[1] F. Krausz and M. Ivanov, *Rev. Mod. Phys.* 81, 163 (2009).

[2] M. Först et al, *Nature Physics* 7, 854–856 (2011)

[3] D. Fausti, et al. *Science* 331, 189–191 (2011)

[4] G. Stefanucci and R. van Leeuwen, *Nonequilibrium Many-Body Theory of Quantum Systems: A Modern Introduction* (Cambridge University Press, Cambridge, 2013)

## 1.2 Number of participants

We expect to have:

- 80 participants, divided in around 30 PDRA and 20 PhD students and 30 experienced researchers.

- Of the 80 participants we expect to have 48 speakers divided in 8 keynote, 16 invited and 24 contributed. The keynote and invited are expected to be experienced researchers. Contributed will be mainly Post-Doctoral Research Associate (PDRA).

## 1.3 Organisers' biography

### Giulio Cerullo

Giulio Cerullo is a Full Professor with the Physics Department, Politecnico di Milano, where he leads the Ultrafast Optical Spectroscopy laboratory. Prof. Cerullo's research activity covers a broad area known as "Ultrafast Optical Science", and concerns on the one hand pushing our capabilities to generate and manipulate ultrashort light pulses, and on the other hand using such pulses to capture the dynamics of ultrafast events in molecules, nanostructures and two-dimensional materials (graphene, transition metal dichalcogenides). Additional research topics are the applications of ultrafast lasers to coherent Raman microscopy and micro/nanostructuring. He has published more than 420 papers which have received more than 17000 citations (H-index: 69, Scopus). He is a Fellow of the Optical Society of America and Chair of the Quantum Electronics and Optics Division of the European Physical Society. He is the recipient of an ERC Advanced Grant (2012-2017) on two-dimensional electronic spectroscopy of biomolecules. He is on the Editorial Advisory Board of the journals *Optica*, *Laser&Photonics Reviews*, *Scientific Reports*, *Chemical Physics*, *Journal of Raman spectroscopy*. He is General Chair of the conferences CLEO/Europe 2017, Ultrafast Phenomena 2018 and the International Conference on Raman Spectroscopy 2020.

### E.K.U. Gross

Scientific Curriculum

Since 2017 Professor of Chemistry, Hebrew University Jerusalem.

Since 2009 Director at the Max Planck Institute of Microstructure Physics, Halle.

2001-2009 Professor of Theoretical Physics at the Free University Berlin.

1990-2001 Fiebigler Professor at University of Würzburg.

1986-1990 Heisenberg Fellow at University of California, Santa Barbara.

1986 Habilitation and *venia legendi*, J.W. Goethe University Frankfurt.

1984-1986 Postdoctoral physicist at University of California, Santa Barbara (with Walter Kohn).

1980-1984 Research assistant at J.W. Goethe University Frankfurt.

1980 Dr. phil. nat., J.W. Goethe University Frankfurt, Physics Department.

### Honors and Awards

- ERC Advanced Grant, 2018.

- Fellow of the American Physical Society, 2017.

- Berni Alder CECAM prize, Lausanne, 2016. Awarded every three years for outstanding contributions to the field of computer simulations in condensed matter physics, statistical physics and physical chemistry. It is the most prestigious European prize in this field and comes with a prize money of 5000 EUR.

- Tsungming Tu Prize, Taipei, 2016. Awarded once a year, this is the highest academic honor granted by the Taiwanese Ministry of Science and Technology to international scholars for outstanding academic achievements. It comes with a prize money of 75,000 USD.

- Senior CMOA Medal for outstanding scientific achievements, 2015.

- Visiting Research Professorship at University of Hong Kong, 2013-2017.

- Elected Max Planck Fellow at the Fritz-Haber-Institut Berlin, 2005-2009.

- Schlumberger Award with medal, Cambridge, UK, 2004.

- Visiting Fellow, Trinity College, Cambridge, UK, 2003-2004.

- Benjamin Meaker Professorship, University of Bristol, UK, 2000.

- International Research Fellow of the Australian Research Council, 1994-1995.

- Heisenberg Fellowship (a highly prestigious young-researcher fellowship of the German Science foundation that allows the recipient to spend up to 5 years at any scientific institution worldwide), 1986-1990.

- NATO Postdoctoral Fellowship, 1984-1985.

- Study Fellowship and PhD Fellowship of the "Studienstiftung des deutschen Volkes". (Federal German foundation for the support of outstanding students), 1973-1979.

- First Prize in the Federal German Mathematics Competition, 1971.

Over 270 articles and book chapters, cited more than 30,000 times

H-Index: 67

More than 370 invited lectures at International Conferences and Colloquia (since 2000)

#### Special lectures

- The 2016 Kenneth S. Pitzer Memorial Lecture, UC Berkeley, October 25, 2016.
- The 2015 CECAM Lecture, EPFL (Switzerland), September 28, 2015.
- Greg Watson Lecture, Rutherford Appleton Laboratory (UK), May 16, 2011.
- Zhong Guan Cun Forum, Institute of Physics, Chinese Academy of Sciences (Beijing), December 19, 2006.
- Pauli Colloquium, University of Vienna (Austria), March 31, 2006.
- Ehrenfest Colloquium, University of Leiden (Netherlands), April 27, 2005.
- Schlumberger Lecture, University of Cambridge (UK), January 15, 2004.
- Benjamin Meaker Lecture, University of Bristol (UK), March 27, 2000.

#### Activities within the Scientific Community (from 2000 onwards)

- Co-organizer of 26 International Workshops, Conferences and Schools.
- Member of the Scientific Advisory Board of NORDITA, Stockholm.
- Member of the Scientific Advisory Committee of CECAM (Centre Européen du Calcul Atomique et Moléculaire), Lausanne, since 2010.
- German (DFG) representative (2003-2009) in the Council of CECAM, president of CECAM Council 2004-2008
- Editorial Board member of the Springer series “Progress in Theoretical Chemistry and Physics”.
- Node coordinator in the EU FP7 Nanosciences, Nanotechnologies, Materials and new Production Technologies Collaborative Project “CRONOS: The dynamics and control in nanostructures for magnetic recording and energy applications”, 2012-2015.
- Steering Committee member of the ESF program “Interdisciplinary Approaches to Functional Electronic and Biological Materials” (INTELBIOMAT) 2008-2013.
- Node coordinator in the EU Infrastructure Initiative: European Theoretical Spectroscopy Facility (ETSF), and member of governing board, 2008-2011.
- Node coordinator in the EU Network of Excellence “NANOQUANTA: Nanoscale Quantum Simulations for Nanostructures and Advanced Materials” (and member of governing board), 2004-2008.
- Node coordinator in the EU Research Infrastructures Action “LIGHTNET”, a theory consortium associated with synchrotron-related research, 2006-2010.
- Node leader (and coordinator of all theory projects) in the EU Research and Training Network “EXC!TING: First-Principles Approach to the Calculation of Optical Properties of Solids”, 2002-2006.
- Node leader (and coordinator of all superconductivity projects) in the EU TMR Network “ $\Psi$ k: Ab initio calculation of complex processes in materials”, 1998-2003.
- Steering Committee member of the ESF program “Electronic Structure Calcul

#### **Andrea Marini**

Dr. Andrea Marini is full time researcher at the Institute for Material Science (ISM) of the National Research Council (CNR). He is mainly involved in the development of novel theoretical approaches and computational tools to describe the ground- and excited-state properties (both at add out of the equilibrium) of complex materials. He is the founder of the YAMBO project, an interdisciplinary and international collaboration for the implementation of a unified tool for the simulation of excited-state properties from first principles. He is now the coordinator of a laboratory (FLASHit) at the ISM-CNR which combine experimental and theoretical methods to investigate ultra-fast and ultra-intense processes at the nano-scale. His group at the CNR-ISM is now member of two H2020 projects (MaX and NFFA). MaX is devoted to the exploration of new numerical methods, in the exascale regime, applied to several fields of physics. NFFA is an European user infrastructure where A.Marini contributes with support to real-time experiments. He is author of 71 publications in international and peer-reviewed scientific journals (with about 3426 citations, h-index=30), and has given a total of 64 invited talks, lectures and seminars.

#### **MAURO NISOLI**

##### PERSONAL INFORMATION:

Family name, First name: Nisoli Mauro

Date of birth: October 11, 1965

orcid.org/0000-0003-2309-732X

URL for web site: [www.attosecond.fisi.polimi.it](http://www.attosecond.fisi.polimi.it)

#### ACADEMIC CARRIER:

From 2011: Full Professor at Politecnico di Milano.

2001 – 2010: Associate Professor at Politecnico di Milano.

1991 – 2001: Researcher of the National Research Council (CNR)

#### FELLOWSHIPS AND AWARDS:

- OSA Fellow 2019: "For innovative contributions to the field of attosecond science and technology, particularly for ground-breaking applications of attosecond pulses to molecules"

- ERC-Advanced Grant (227355 – ELYCHE) 2009 – 2014

#### RESEARCH FOCUS

Attosecond science and technology. Ultrafast phenomena in atomic and molecular physics, with temporal resolution down to the attosecond regime. Ultrashort-pulse laser technology. Atomic and molecular physics. Extreme nonlinear optics. Atoms in strong laser fields. Applications of femtosecond light pulses to the investigation of ultrafast processes in organic and inorganic semiconductors and nanostructures. Optical parametric processes for the generation of few-optical-cycle pulses.

#### PATENT

United States Patent 5956173: Capillary compressor (Inventors: S. De Silvestri, M. Nisoli and O. Svelto).

#### BIBLIOMETRICS

He is author of 188 research papers in international journals. H-index (Scopus): 49.

He has given about 100 invited and tutorial communications at international meetings and schools. He is co-author of didactic books of Physics and Quantum Electronics. He is reviewer for several international scientific journals

#### ORGANISATION OF SCIENTIFIC MEETINGS

2013: General Chair – CLEO-Europe (Conference on Lasers and Electro-Optics), Germany

2011: Program Chair – CLEO-Europe (Conference on Lasers and Electro-Optics), Germany

2010: Co-Chair – ISUILS9 (International Symposium on Ultrafast Intense Laser Science), U.S.A.

2008: Local Chair – XVI International Conference on Ultrafast Phenomena, Italy.

#### COORDINATION OF RESEARCH NETWORKS

2012 – 2015 Scientific Coordinator for the European CUSBO facility of the European "Joint Research Activity" JRA-INREX (Innovative radiation sources at the extremes)

2009 – 2012 Scientific Coordinator for CUSBO facility of JRA-ALADIN (Attosecond laser sources and applications; design and innovation)

2006 – 2009 Scientific Coordinator for CUSBO facility of JRA-FOSCIL (Frontiers of Optical Science: Controlling Intense Light)

2008 – 2012 Coordinator of the Italian node of the Marie Curie Research Training Network Ultrafast dynamics using attosecond and XUV Free Electron Laser sources (ATTOFEL) FP7-238362

2004 – 2008 Coordinator of the Italian node of the Marie Curie Research Training Network Ultrashort XUV Pulses for Time-Resolved and Non-Linear Applications (XTRA) MRTN-CT-2003-505138

#### COMMISSIONS OF TRUST

2013 Member of the Appointment Committee by the Chemistry, Physics and Technology Section (CPTS) of the Max Planck Society's Scientific Council

2013 – Member of William F. Meggers Award Committee (Optical Society of America)

2008 – Co-Editor Applied Physics B: Lasers and Optics

2009 – Reviewer for Department of Energy (DOE) – Basic Energy Sciences (BES)

2006 – Reviewer for Netherlands Organisation for Scientific Research (NWO)

2006 – Reviewer for U.S. - Israel Binational Science Foundation

2004 – Reviewer of PhD thesis (member of the jury) at: ETH Zurich (Switzerland); Imperial College, London (UK); Université Paris-Sud (France).

### **Angel Rubio**

EDUCATION: Male, born 27.09.1965 in Oviedo, Spain

University of Valladolid, Spain, Ph.D. in Physics, “Summa Cum Laude”, 1991.

University of Valladolid, Spain, B.S. in Physics, “Summa Cum Laude”, 1988.

#### SCIENTIFIC CAREER:

Max-Planck Distinguished Visiting Scientist, Fritz Haber Institute MPG Berlin (2009-2011)

Miller Visiting Professor, University of California at Berkeley (August-September 2014)

Full Professor of Condensed Matter Physics (chair), UPV/EHU (since April 2001-Dec.2014)

Chair of the European Theoretical Spectroscopy Facility (ETSF) (<http://www.etsf.eu>) (since 2012-) and Vice-President for Scientific Development (since 2008)

Director of Nano-bio Spectroscopy group of the UPV/EHU (since 2002-)

Professor (1ere class), Universidad de Montpellier 2, Francia, (June-July 2007).

Professor (Humboldt), Freie Universitat Berlin, 2005/2006.

Professor, Laboratoire des Solides Irradiés, Ecole Polytechnique, France. (Dec.2000-Apr.2001).

Associate Professor, Dpt. Física Teórica, Atomica y Nuclear, Universidad Valladolid, 1994-2001

Fulbright Fellow, Department of Physics, University of California at Berkeley, USA. (1992-1994)

Research Fellow “Ministerio de Educación y Ciencia”, Universidad Valladolid. Spain (1988-92)

#### HONORS / AWARDS:

Medal of the Spanish Royal Physical Society 2016

European Research Council “ERC Advanced Grant” (2016 - 2021) (QSpec-NewMat)

Member of the Academia Europaea (2016)

XV Manuel Laborde Werlinden Prize for the best technology-based business initiative based on innovative ideas: "Materials Evolution", December 2015

Premio Jaime I de Investigación Básica 2014.

Foreign associate member of the National Academy of Sciences (NAS) of United States (2014)

External Scientific Member of the Fritz-Haber-Institut-Max-Planck-Gesellschaft, (Nov. 2011-)

European Research Council “ERC Advanced Grant” (2011-2016) (DYNamo)

Fellow of the American Association for Advanced Science (AAAS) (Physics Section) (2010)

Dupont Prize in Nanotechnology, Dupont Foundation (2006)

Friedrich Wilhelm Bessel Research Award, Humboldt Foundation (2005)

Fellow of the American Physical Society, Division of Materials Science (2004)

Spanish Royal Physical Society Prize “Jóvenes Investigadores” Madrid. Spain. July, 1992

Honor Prize for the best Ph.D. Thesis in Physics University of Valladolid. Spain. June, 1992.

1st National Prize for Graduated in Physics October 25, 1989

#### SCHOLARLY CONTRIBUTIONS:

More than 300 publications with over 25000 ISI Web of Science (H-index=79; 2,000 cites per year and growing).

Note that 36 of his publications are ranked as “Highly Cited Papers”

Director of 30 PhD students (12 running); supervisor of 45 postdoctoral researchers. Twelve of my former graduate students and twenty-nine of the postdocs now hold academic positions at major universities worldwide. Four other students now hold leading positions in the industry.

More than 180 invited talks, 40 Colloquium; numerous outreach talks and press releases.

Originator of the widely-used ab initio computational materials research open-source project octopus

(<http://www.tddft.org>). It simulates the dynamics of electrons and nuclei under the influence of time-dependent field, used by more than 600 groups worldwide.

#### PATENTS:

Gated-controlled light-emitting device made of BN nanotubes with defects, UPV/EHU (2011); (201130228, ID02207561); US-2014-0014900-A1)

Field emission source with BN nanotubes, Universidad de Valladolid, P-9802690 (2001).

### **Gianluca Stefanucci**

Dr. Gianluca Stefanucci got his PhD in 2002 with a work on the pairing mechanism

in high  $T_c$  superconductors and on the antiferromagnetic order of strongly correlated lattice systems. He found the first analytic solution with antiferromagnetic order in a Hubbard-like model. In 2003 Dr. Stefanucci moved to Lund University (Sweden) to work in the field of quantum transport and fundamentals of TDDFT. He formulated a Green's function theory as well as a TDDFT scheme to deal with transient responses and other time-dependent phenomena. In this period he also formulated an algorithm for numerical quantum transport simulations. In 2006 Dr. Stefanucci moved to the Freie Universitat of Berlin where he continued to work in the field of time-dependent quantum transport, and in year 2007 he got a permanent researcher position in Rome at the University of Tor Vergata. In Rome the research activity of Dr. Stefanucci expanded toward molecular photovoltaics, spintronics, Josephson nanojunctions, nanojunctions with Kondo correlations and in the Coulomb blockade regime, inelastic quantum transport, low-dimensional systems and Luttinger liquids, and more recently transient spectroscopy and thermal transport. He also contributed to the formal development of Green's function theory with a work on Kadanoff-Baym equations in open systems, on the Wick theorem for general initial states and a new diagrammatic expansion for Green functions and response functions with positive spectral properties. In 2013 he co-authored with Prof. R. van Leeuwen a book published by Cambridge University Press on Nonequilibrium Green's functions and Many-Body Theory. Dr. Stefanucci gave about 40 invited talks, 15 invited seminars in research institutes and universities and he is author of 100 publications (~25 with only one coauthor, h-index 24, total number of citations > 2000).

## 2 Participant List

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### Organizers

#### **Cerullo Giulio**

Polytechnic University of Milan, Italy

#### **Gross E.K.U.**

Max Planck Institute of Microstructure Physics, Halle

#### **Marini Andrea**

National Research Council

#### **NISOLI MAURO**

Politecnico di Milano

#### **Rubio Angel**

Max Planck Institute for the Structure and Dynamics of Matter

#### **Stefanucci Gianluca**

University of Rome, Tor Vergata, Italy

#### **Biegert Jens**

ICFO (Barcelona, Spain)

*Positive response received*

#### **Burghardt Irene**

Goethe-Universität Frankfurt, Germany

*Positive response received*

**Ernstorfer Ralph**

Department of Physical Chemistry Fritz-Haber-Institut, Berlin

*Positive response received*

**Hauer Jürgen**

Technical University of Munich

*Positive response received*

**Leitenstorfer Alfred**

Department of Physics University of Konstanz

*Positive response received*

**Tavernelli Ivano**

Zurich Research Laboratory, Zurich, Switzerland

*Positive response received*

**Vrakking Marc**

Max Born Institut (Berlin, Germany)

*Positive response received*

**Werner Philip**

University of Fribourg, Switzerland

*Positive response received*

## 3 Financial support

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### Supports

**Overall budget :** 30000€

**CECAM contribution :** 15000€

**PsiK contribution :** 15000€

### Financial remarks

The requested budget is of around 30000 Euro. Based on our past experience in organizing a conference in the same location we can give a first but rather accurate estimation of the budget components:

Accommodation: 7680 Euro (calculated for invited and keynote speakers at 80 Euro per night)

Coffee breaks: 3360 Euro (calculated at 6 Euro per person for 80 participants, 7 breaks)

Dinner: 3200 Euro (calculated at 40 Euro per person for 80 participants)

Travel: 12000 Euro (calculated at max 500 Euro per participant for the 24 keynote and invited speakers)

Poster Session: 1120 Euro (calculated at 14 Euro per person for 80 participants)

Bursaries: we plan to give to 10 PDRA/PhD students a 300 Euro bursary each to contribute to the conference costs.

This result in an additional 3000 Euro.



Total: 30000 Euro