

# **CECAM (Centre Européen de Calcul Atomique et Moléculaire)**

## **Activities' Report - Year 2016**

**Filippo De Angelis**

### **1. Introduction**

CECAM (European Center for Calculating Atomics and Molecules, <http://www.cecaml.org/>) is a European organization that promotes frontier research in the computational sciences. The focus of CECAM are atomistic and molecular simulations applied to the physics and chemistry of condensed matter, to materials science and to biological and medical chemistry. CECAM is organized in a district headquarters (EPFL) in Lausanne, Switzerland, and has 18 nodes across the various participating countries. Below is a list of nodes with the countries of affiliation:

- [CECAM-AT](#)
- [CECAM-FI](#)
- [CECAM-FR-MOSER](#)
- [CECAM-FR-RA](#)
- [CECAM-FR-GSO](#)
- [CECAM-DE-MMIP](#)
- [CECAM-DE-JUELICH](#)
- [CECAM-DE-MMS](#)
- [CECAM-DE-SMSM](#)
- [CECAM-IRL](#)
- [CECAM-ISR](#)
- [CECAM-IT-SIDE](#)
- [CECAM-IT-SMART](#)
- [CECAM-IT-SIMUL](#)
- [CECAM-NL](#)
- [CECAM-ES](#)
- [CECAM-UK-HARTREE](#)
- [CECAM-UK-JCMAXWELL](#)

The italian nodes are: SIMUL - Istituto Italiano di Tecnologia (IIT), SMART - Scuola Normale Superiore (SNS) and SIDE - Scuola Internazionale Superiore di Studi Avanzati (SISSA).

### **2. Main activities carried on by CECAM during 2016 relevant for Italy and for CNR**

Italy participates in the CECAM Council with four Institutions, CNR and the three node-related Institutions IIT, SNS and SISSA. Italy is in fact the country with the largest number of Institutions in the CECAM Council. During the year 2017 a fifth Italian Institution will join CECAM, the University of Bologna.

The activities of CECAM are carried out through the scientific actions of the nodes and through the organization of international workshops, schools and conferences. CECAM provides an average support of €12,000 per event, as well as logistical and organizational support (secretarial, Web pages, contact management, hotel booking, etc.).

In 2016 50 workshops were organized, 6 of these events were organized by CNR researchers on a total of 9 events organized by Italian Institutes. One further workshop was organized in Italy European researchers (see Appendix A).

For the year 2017, 33 workshops have been planned or have already been carried out, 10 Italian researchers (3 CNR) are among the organizers of 10 of these events. Most notably, the only CECAM conference planned for 2017 is organized by a CNR researcher, see Appendix A. There are also numerous CNR researchers among the invited speakers and participants in CECAM initiatives.

In 2016, 18 schools were organized, 3 were organized by Italian researchers and 1 was organized by CNR researchers, Appendix A.

### **3. Activities carried out within the Union during 2016 and impact on the Italian scientific community**

During 2016 both myself and Silvia Picozzi (second CNR delegate at CECAM) attended as CNR representatives the CECAM Council Meetings, held at the headquarters in Lausanne on 22/04/2016. I have attended also the 24-25/11 CECAM Council meeting, held in Lausanne. In the meeting held in April the new CECAM Director, Prof. Ignacio Pagonabarraga, was appointed.

In the second meeting we discussed the financial lines for 2017-2018 and the activities carried out in 2016 were evaluated. Following the explicit proposal of the undersigned, it was agreed to reduce the CNR participation fee of 50,000 Euros (historically paid by CNR) to 30,000 Euros per year, homogenizing the fee to that of the other institutions, with considerable savings for the CNR. This reduction has no impact on CNR's activities and presence.

With the contrary vote of the undersigned, it was extended to Australian Institutions (US institutions did not respond) to become members of the CECAM. I have reaffirmed that the CECAM is a European institution, and I therefore proposed that non-European countries should be admitted as "associated countries" and not as members.

Professor Alessandrio Laio, SISSA, Trieste and CNR-DEMOCRITOS was appointed as CECAM President.

The call for workshop proposals for the year 2018 is currently open, <http://www.cecarn.org/submitting.html>. To encourage the widest possible participation by CNR staff, several messages have been sent to the scientific community, providing information and supporting the proposals.

### **4. Evaluation of the participation in terms of benefits and membership cost**

The CNR presence in CECAM is important to maintaining and strengthening Italy's weight in the European computational community, which in fact is largely identified in CECAM as its main organization and representative body. From a strictly cost/benefit point of view, 6 workshops would imply a budget of 70,000 Euros, against a fee of 50,000 Euros, now updated to 30,000 Euros. It is therefore obvious that the economic benefits from access to funds are clearly in favor of CNR staff. By supporting CECAM, CNR has the opportunity to further strengthen its weight in scientific calculations and simulations, launching initiatives in areas of interest between physics, materials science and chemistry as well as biological and medical chemistry. These activities are widely recognized at the European level and many call for proposals in the H2020 program are inherent to computational science, modeling and simulation. Recently CECAM coordinated the presentation of European initiatives that attracted considerable funding, such as the E-CAM project. This project, funded by H2020, aims to create an electronic infrastructure (e-infrastructure) dedicated to software development, training and consulting in modeling and simulation. CNR's participation at CECAM can also be an opportunity to access to European funding otherwise difficult to access to the single researcher operating in modeling and simulation.

### **5. Evaluation of Italians' attendance and how to improve interest and involvement**

There was a general reluctance from CNR staff not previously involved in CECAM initiatives to apply for workshops funded by CECAM, despite the wide publicity through institutional channels and personal contacts by the undersigned. I personally consider very important to highlight this opportunity by linking the call for proposals in the CNR Departments websites and in the Institutional website.

### **6. Italian experts with important roles within the Union or within related Commissions and Programs (if known)**

The deputy director of CECAM is Dr. Sara Bonella, Università di Roma La Sapienza.

The new president of CECAM is Prof. Alessandro Laio, SISSA and CNR-DEMOCRITOS.

### **7. If Union with CNR Commission, short summary about the 2016 CNR Commission activities**

N/A

## 8. Notes (if any)

N/A

## 9. Conclusions

CECAM is set up as European reference in modeling and computational simulation activities, recognized in major H2020 calls as a center for scientific and technological development. The CNR's participation to CECAM is strategic as it allows our staff to be represented at the decision-making venue and to have access to funding for organizing workshops. With the entry of a new Italian partner in 2017, Italy will be the country with the largest number of member institutions, thus being able to pursue a positive synergy for the Italian research system. I fully supports the continuation of CNR's participation in CECAM.

Signature

A handwritten signature in blue ink, appearing to be 'G. U. L.', is written below the 'Signature' label.

Perugia, 15/05/2017

Please return as pdf to: [virginia.codanunziate@cnr.it](mailto:virginia.codanunziate@cnr.it), [cecilia.lalle@cnr.it](mailto:cecilia.lalle@cnr.it) before May 15<sup>th</sup>, 2017

## Appendix A

### Participation of researchers belonging to Italian Institutions to CECAM activities in 2016 (highlighted are those activities organized by CNR staff)

#### Conferences.

##### Ab initio Spin-orbitronics

Location : The conference will take place in the area of Pescara/Montesilvano (Italy)

*September 25, 2017 - September 29, 2017*

- Silvia Picozzi  
Consiglio Nazionale delle Ricerche CNR-SPIN, Chieti, Italy
- Stefan Blügel  
Forschungszentrum Jülich, Germany
- Ingrid Mertig  
Martin Luther University Halle, Germany

#### Workshops.

##### Hydrodynamic Fluctuations in Soft-Matter Simulations (organizzato in Italia ma non da ricercatori Italiani)

Location : Monash University Prato Centre, Italy, see <http://www.ita.monash.edu/>

*February 9, 2016 - February 12, 2016*

- Burkhard Duenweg

Max Planck Institute for Polymer Research, Mainz, Germany

- Ravi Prakash Jagadeeshan

Monash University, Melbourne, Australia

- Friederike Schmid

Johannes Gutenberg University, Mainz, Institute of Physics, Germany

##### 1) Ultra-fast phenomena in quantum physics: a challenge for theory & experiment

Location : CECAM-HQ-EPFL, Lausanne, Switzerland

*April 11, 2016 - April 15, 2016*

- Andrea Marini  
National Research Council, Italy
- Gianluca Stefanucci  
University of Rome, Tor Vergata, Italy, Italy
- Cristian Manzoni  
IFN-CNR Dipartimento di Fisica, Politecnico di Milano, Italy
- Deborah Prezzi  
CNR-NANO, Modena, Italy

##### 2) Marrying continuum and molecular physics: the Andersen-Parrinello-Rahman method revised into a scale bridging device

Location : CECAM-HQ-EPFL, Lausanne, Switzerland

*May 23, 2016 - May 26, 2016*

- Antonio DiCarlo  
CECAM-IT-SIMUL Node, Italy
- Giovanni Ciccotti  
University of Rome La Sapienza, Italy

##### 3) Structural and Functional Annotation of Bioinorganic Systems: Perspectives and Challenges from Theory and Experiments

Location : CECAM-IT-SNS

*May 23, 2016 - May 25, 2016*

- Giuseppe Brancato  
Scuola Normale Superiore, Pisa, Italy

- Vincenzo Barone  
Scuola Normale Superiore Pisa, Italy
- Paolo Carloni  
German Research School for Simulation Sciences Julich, Germany
- Alessandra Magistrato  
CNR-IOM@SISSA, Italy
- Giuseppe Legname  
Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy
- Rachel Nechushtai  
Hebrew University of Jerusalem, Israel, Israel

#### **4) Different Routes to Quantum Molecular Dynamics**

Location : CECAM-HQ-EPFL, Lausanne, Switzerland

*June 6, 2016 - June 10, 2016*

- Basile Curchod  
University of Bristol, United Kingdom
- Michele Ceotto  
Università degli Studi di Milano, Italy
- Guillermo Albareda  
Universitat de Barcelona, Spain
- Ali Abedi  
University of Basque Country, Spain
- Philipp Marquetand  
University of Vienna, Austria

#### **5) Atomistic simulations in prebiotic chemistry – a dialog between experiment and theory**

Location : CECAM-FR-IDF, University Pierre and Marie Curie, Paris, France

*June 20, 2016 - June 22, 2016*

A. Marco Saitta  
University Pierre and Marie Curie, Paris, France  
Fabio Pietrucci  
UPMC - Sorbonne Paris, France  
Judit Sponer  
Institute of Biophysics, Brno, Czech Republic  
Franz Saija  
Istituto per i Processi Chimico-Fisici - CNR, Italy  
Rodolphe Vuilleumier  
Ecole Normale Supérieure, Paris, France

#### **6) Nonequilibrium Statistical Mechanics and Turbulence**

Location : CECAM-IT-SIMUL

*September 8, 2016 - September 10, 2016*

Carlo Massimo Casciola  
University of Rome I "La Sapienza", Italy  
Sergio Chibbaro  
Pierre et Marie Curie University, France  
Lamberto Rondoni  
Politecnico di Torino, Italy

#### **7) Interface processes in photochemical water splitting: Theory meets experiment**

Location : CECAM-HQ-EPFL, Lausanne, Switzerland

*September 27, 2016 - September 30, 2016*

- Mariachiara Pastore  
CNRS, France & CNR-ISTM, Perugia
- Ilaria Ciofini  
CNRS, France
- Stefano Fabris  
CNR-IOM DEMOCRITOS Simulation Center and SISSA, Trieste, Italy
- Simone Piccinin  
CNR-IOM DEMOCRITOS Simulation Center, Trieste, Italy

### **8) Molecular chirality from a physical and theoretical chemistry perspective**

Location : CECAM-HQ-EPFL, Lausanne, Switzerland

*October 10, 2016 - October 12, 2016*

- Andrea Lombardi  
University of Perugia, Italy
- Federico Palazzetti  
University of Perugia, Italy

### **9) Computational methods towards engineering novel correlated materials**

Location : CECAM-HQ-EPFL, Lausanne, Switzerland

*October 24, 2016 - October 26, 2016*

- Markus Aichhorn  
Institute of Theoretical and Computational Physics, University of Technology Graz, Austria
- Gianluca Giovannetti  
CNR-IOM and Sissa, Italy
- Philipp Hansmann  
Max Planck Institute for Solid State Research, Germany

## **Schools.**

### **1) SMART Winter School (Space-time Multiscale Approaches for Research and Technology)**

Location : CECAM-IT-SNS

*January 25, 2016 - January 29, 2016*

- Vincenzo Barone  
Scuola Normale Superiore, Italy
- Benedetta Mennucci  
University of Pisa, Italy
- Ilaria Ciofini  
CNRS, France
- Malgorzata Biczysko  
Shanghai University, China

### **2) Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology, and Biophysics**

Location : CECAM-IT-SIDE

*July 5, 2016 - July 22, 2016*

- Federico Becca  
International School for Advanced Studies (SISSA) and CNR-DEMOCRITOS IOM, Italy
- Alessandro Laio  
International School for Advanced Studies (SISSA), Trieste, Italy
- Angelo Rosa  
International School for Advanced Studies (SISSA), Trieste, Italy

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