

# 2nd NOMAD (Novel Materials Discovery) Industry Workshop



**Proposed dates :**

*Feb 06, 2017 - Feb 07, 2017*

**Alternative dates :**

*Feb 06, 2018 - Feb 07, 2018*

**Alessandro De Vita**

*King's College London and University of Trieste*

**Matthias Scheffler**

*Fritz Haber Institute of the Max Planck Society (FHI), Berlin*

**Angel Rubio**

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

# 1 Proposal

---

## 1.1 State of the art

Virtually every new commercial product, be they smart phones, solar cells, batteries, transport technology, artificial hips, etc., depends on improved or even novel materials, which makes materials discovery highly relevant for research and industry. Computational materials science is an increasingly influential method to identify such critical materials for industrial R&D. Enormous amounts of data, precious but heterogeneous and as such difficult to access and utilize, are already stored in repositories scattered across Europe.

The Novel Materials Discovery (NOMAD) Laboratory [1] was recently founded by a team of computational materials science groups with complementary expertise, and a few high-performance computing centers, to open new HPC opportunities by enabling data access and delivering powerful new tools to search, retrieve and manage it. The objectives of this European Center of Excellence (CoE) include the creation of a materials encyclopedia, and the development of big-data analytics and advanced graphics tools for materials science and engineering. Those goals are complementary with those of the other two CoEs supported by the European Commission and active in the field of CECAM activities (E-cam [2] and Max [3]). The NOMAD Researchers are currently creating a large, homogenised materials database, as well as the analytical tools and code developments necessary to extract information from it. We are confident that the available HPC infrastructure and the envisaged developments will contribute to the discovery of new scientific phenomena, novel devices, and advances in materials science and engineering. An essential corner stone of the project is the NOMAD Repository [4] which contains the produced data and records the input and output files of many high-quality calculations performed fellow researchers working all over the world. The Repository is unique in the sense that it is not restricted to one or a few simulation programs ("codes") but it accepts output from all important codes. As of early July 2016, it contains results from more than three million different calculations, corresponding to billions of CPU-core hours used on several high-performance computers all over the planet. Recently, there has been a very significant growth of industrial interest (from large companies as well as SMEs) in computational materials science, motivated by the innovation potential of new materials and improved existing materials. However, the scientific complexity of the topic and the heterogeneous and fragmented nature of the research field make it difficult to translate research leadership into accomplished innovation.

Thus, it is particularly important at this point in time to bring materials modelling closer to industrial/societal exploitation in real terms. We strive to establish among EU-based industries full awareness of the extent to which the wealth of newly available data could boost their competitiveness. To raise industrial interest, the potential of big-data activities to foster industrial business will have to be made apparent in practical terms. We believe that this requires close engagement with industries already at the tool design level. We are also convinced that workshops with industry representatives are important (in fact, indispensable) venues to gather industrial feedback on their plans and needs concerning materials data, and to inform/train industry representatives on tool-usage for industrial R&D users. The workshop proposed here will accomplish both of these goals.

### References

- [1] <https://nomad-coe.eu/>
- [2] <http://www.e-cam2020.eu/>
- [3] <http://www.max-centre.eu/mission/>
- [4] <http://nomad-repository.eu/cms/>

## 1.2 Description

To create a sensible baseline for discussion among all participants, the workshop will start with NOMAD researchers introducing the goals of the CoE, and providing an update on the current status of the project.

This introduction will outline the objectives and activities of the NOMAD initiative as a whole, emphasizing how this is not limited to the big-data "four Vs" (i.e., data curation in terms of optimising and monitoring data volume, variety, velocity, and veracity), but rather aims to deliver to users an analytics toolkit geared for practical data usage. This marks one of the differences between NOMAD and, e.g., the US Materials Genome Initiative, where

analytics does not play a noticeable role, so far. The status of the Repository and the progress of the conversion layer of different codes will also be discussed briefly.

We will then bring to the discussion the central theme of industry networking, focusing on identifying optimal strategy to enhance the interaction of industry with academic materials modelling data-based research. We expect this to examine means to gather information on identifying industrial needs via interviews, workshops, hands on sessions, eventually followed by the design and realisation of case studies. Usability (user friendly interface) of the data tools planned by the CoE, and appropriate action to raise awareness of their availability are other important issues we expect to be addressed and discussed.

The introductory session will be followed by a further “Where are we now?” section where the goals and status of the different parts of the NOMAD project will be described and discussed, together with the challenges that lie ahead. This will describe the NOMAD Encyclopedia which is the primary tool allowing access to the wealth of information stored within the database. In fact, the encyclopedia will enable access to information through a materials search engine, which will be made available to everyone as an open access tool.

Two more short technical talk will follow, introducing tools planned by the CoE but not yet available at the time of the workshop. (1) We will first introduce the big-data analytics toolkit with examples of the functionalities that the CoE aims to provide to boost the exploitation of the materials database. This will discuss searching tools suitable to explore the explosively big materials configuration basin, and how big-data analytics techniques could help detect hidden “game changers”, speeding up the process of discovery of novel candidate materials for real life applications. (2) We will then describe the graphics tools planned in the CoE, based on remote visualization through a web-like interface (so that no download will be required). Virtual reality will also be discussed as an aid tool for interacting with with complex, high-dimensional data sets.

The above will be followed by a main session during which three key industry representatives will lay out their specific needs and plans for computational materials science in general and their expectations for this (type of) initiative in particular.

A fourth session on the second day will consist of two general panel discussions on

- Industry Wish List, and
- Interaction with industry (on feedback gathering, software training, case studies,...)

We expect this discussion to provide useful feedback on how to shape the industry networking activities of this (and any similar) initiative, making it more relevant for industry users.

The workshop will conclude with a summary of the discussion and its outcomes.

The workshop will be held at the Center for Free-Electron Laser Science in Hamburg.

## 1.3 Timetable

Day 1 – 06 Feb 2017

- 14:00 Registration, coffee
- 15:30 Welcome and general introduction (Matthias Scheffler)

Session I: Interaction with Industry

- 15:50 The Nomad Industry Networking (Angel Rubio, Alessandro De Vita)

Session II: Where are we now?

- 16:00 The Materials Encyclopedia (Claudia Draxl)
- 16:10 A data analytics toolbox (Luca Ghiringhelli)
- 16:20 Advanced graphics (Rubén Jesús García Hernández)

Coffee Break and Networking

Listening to Industry Needs

- 17:00 Industry Rep #1

- 17:30 Industry Rep #2
- 18:00 Industry Rep #3
  
- 19:30 Dinner

Day 2 – 07 Feb 2017

- 9:00 Coffee
- 9:15 General Discussion I: Industry wish list (all participants)
- 9:30 General Discussion II: Interaction with Industry (on feedback gathering, software training, case studies,...)
- 10.15 Summary of Actions (Angel Rubio)
- 10.45 Wrap Up and Farewell (Matthias Scheffler)
- 11:00 Meeting ends

## 1.4 Previous workshops

NOMAD: first industrial meeting  
Berlin, Germany  
March 1-2, 2016

## 1.5 Previous CECAM workshops

-

## 1.6 Size of event

We expect 60 participants, about half of whom from industry. This size will allow us to host representatives from a large range of industry sectors who will be able to give us feedback from different angles during the keynote talks and discussion sessions. At the same time, this is still small enough to carry out a meaningful choral discussion.

## 1.7 Organisers' biography

### **Alessandro De Vita**

Professor Dr. Alessandro De Vita PhD (Physics), PhD (Materials Engineering)

Contact:

King's College London

Department of Physics

Research Group: Theory & Simulation of Condensed Matter

Strand, London, WC2R 2LC, UK

Tel + 44 (0) 207 848 2715

e-mail [alessandro.de\\_vita@kcl.ac.uk](mailto:alessandro.de_vita@kcl.ac.uk)

Short Bio:

Alessandro has over twenty-five years experience in materials modelling, which started with a Physics MSc in Trieste, Italy, and developed interdisciplinary spanning over Physics and Materials Engineering, with a PhD in either discipline. During his career he has been working in various UK and EU institutions, including the Universities of Keele, Oxford and Cambridge, the Swiss Federal Institute of Technology (EPFL) in Lausanne, and the University of Trieste. In 2010 he became Professor of Physics at King's College London, where since 2011-2016 he also served as Chair of the Assessment Board (Postgraduate) of the Faculty of Natural and Mathematical Sciences. He is a Scientific Advisory Committee member of the EU Psi-K Network for which has been WG5-“Hybrid Classical and Quantum Methods” Spokesman (2003-2008). He is the KCL Director and former Chair of the Thomas Young London Center for Theory and Simulation of Materials, which he co-founded in 2006. In 2012 he co-founded the UK-JCMaxwell-CECAM Node, coordinating EU-wide scientific events organised by the London Colleges and the universities of Oxford and Cambridge. He became UK-JCMaxwell node director in June 2016.

#### Research:

Alessandro has been a pioneer of large scale parallel computing calculations using electronic structure techniques, which led him to author e.g., first examples of large-scale First Principles MD calculation using the DFT plane-wave formalism on parallel supercomputers and of surface chemical reactions investigations using the First-Principles MD approach. His current research interests are centred on the development and application of information-efficient data-intensive atomistic modelling techniques, notably including the “Learn On The Fly” multi-scale scheme, recently extended to combine Machine Learning with first-principles molecular dynamics and massively parallel computing. He uses these techniques to investigate the origin of the chemo-mechanical properties of materials, such as their resistance to fracture, and pioneered the use of electronic structure based dynamical simulations to study stress corrosion. He furthermore investigates interface properties and surface reactions, notably including nanofabrication by supramolecular self-assembly.

#### Positions:

2010– Professor of Physics, King’s College London, UK  
2005– Professor of Science and Technology of Materials, University of Trieste  
2004– Reader in Physics, Physics Department, King’s College London, UK.  
1998– Lecturer in Chemical Foundations of Technology, University of Trieste, Italy.  
1994– 2002 Senior Research Assistant at the IRRMA/EPFL institute, Lausanne, Switzerland.  
1992– PDRA, Theory of Condensed Matter (TCM) group, Cavendish Laboratory, University of Cambridge, UK, on a joint position with the Earth Sciences Dept., University of Oxford.  
1990– Research Fellow, Physics Department, Keele University, UK.  
1989– MSci in Physics (summa cum laude), Univ. of Trieste, Italy.

#### Angel Rubio

Director. Max Planck Institute for the Structure and Dynamics of Matter (MPSD)  
Luruper Chaussee 149, 22761 Hamburg, Germany

Distinguish Professor: Condensed Matter Physics

Dpt. Física de Materiales, Facultad de Químicas, UPV/EHU, San Sebastián, Spain

Homepage: <http://www.mpsd.mpg.de/113438/theod> ; [http://nano-bio.ehu.es/angel\\_rubio](http://nano-bio.ehu.es/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:

- Professor University of Hamburg (since May 2016-)
- 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), University of the Basque Country UPV/EHU (since April 2001-)
- 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 (Iere 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:

- 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
- American Chemical Society (ACS) recognition (2011) and Outstanding Referee, American Physical Society (2009)
- Sir Allan Sewell Fellowship, Australia, 2004
- JSPS Fellow, Program for Research in Japan, 2001
- Fulbright Fellow, 1992-94

#### SCHOLARLY CONTRIBUTIONS:

- More than 300 publications with over 25000 ISI Web of Science (h-index=76; over 2,000 cites per year and growing). Note: 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 in and outside Spain (Germany, Italy, Austria, Denmark, France, USA, Japan). 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).

#### SELECTED PROFESSIONAL AND SYNERGISTIC ACTIVITIES (recent)

- Selection committee member for the Hamburg Prize for Theoretical Physics 2016
- Member of the judging panel for the CECAM Berni J. Alder prize 2016
- Member of the Scientific Advisory Committee of CECAM (Centre Européen du Calcul Atomique et Moléculaire), Lausanne (2015-) and of the Scientific Council of ZCAM ("Zaragoza Scientific Center for Advance Modeling") (2013-)
- Member of the 2015 Tsungming Tu Award, Ministry of Science and Technology, Taiwan
- Member of the Editorial Board of ChemPhysChem (2015-)
- Editor in Chief of the European Physical Journal B (since July 2011-)
- Panel Member for the Francqui Prize, Belgium (2015)
- Member of the "Centro de excelencia en Nanociencia Molecular ISIC-NANO", Valencia (2012-)
- Panel member of the European Research Council, ERC Starting Grant 2013 PE4 (Physical and Analytical chemical Sciences); Referee for the ERC since 2008- to date
- Member of the Editorial Board of Lecture Notes in Physics, Springer (2011-)
- Referee for the Academy of Finland Academy Professor evaluation (2011-)
- Panel member Prize Polish Foundation for Science in Chemistry and Material Science (2013-)
- Panel member of the Deutsche Forschungsgemeinschaft "Excellence Initiative" (Physics, Mathematics, Geosciences) (2011-)
- Scientific Advisory Board, Centro de Física Computacional Coimbra, Portugal (2011-)
- Scientific Advisory Board, Leibniz-Institut IFW-Dresden (2008, 2011)
- Advisory Board Member and Physical Scientist associated to the ITR: Institute for the Theory of Advanced Materials in Information Technology (ITAMIT), University of Minnesota, since 2003.
- External Advisory Board Member of The center for Nanotechnology and Molecular Materials, Wake Forest University, North Carolina, USA (Director Prof. D.L. Carroll), since 2007.
- Member of the BIFI "Instituto de Biocomputación y física de sistemas complejos", Zaragoza, Spain, since January 2008.

- Member of the Board of Directors of the Psi-k: UK Charity Commission (Psi-K-1126308) and founded director of psi-k.org.
- European Science Foundation (ESF) Pool of Reviews 2008.
- Adviser and referee to European Union "Information Science and Technology Program (2000-).
- Organizer of more than 50 International Workshops and Schools.
- He is one of the founding directors of the European Theoretical Spectroscopy Facility (ETSF) (<http://www.etsf.es>) where he is now the Vicepresident for Scientific Development. T

### **Matthias Scheffler**

Born 1951 in Berlin, Germany

Director at the Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin

Homepage: [www.fhi-berlin.mpg.de/th](http://www.fhi-berlin.mpg.de/th)

Major Research Areas:

Physical and chemical properties of surfaces, interfaces, clusters, and nanostructures, in particular multi-scale studies linking first principles electronic-structure theory, molecular dynamics, and methods from thermodynamics and statistical mechanics. Emphasis is also put on developments beyond density-functional theory (GW, EX+cRPA, vdW).

### Scientific Curriculum

1978 Dr. rer. nat., Technical University Berlin, Physics Department

1978-1987 Scientific staff member of the Physikalisch Technische Bundesanstalt, Braunschweig

1979-1980 Postdoc at the IBM T.J. Watson Research Center, Yorktown Heights

1984 Habilitation and *venia legendi*, Technical University Berlin

Since 1988 Director at the Fritz Haber Institute of the Max Planck Society, Berlin, and Scientific member of the Max Planck Society

Since 2005 Distinguished Visiting Professor at the University of California, Santa Barbara

Since 2010 Member of the board of directors of the 'Max Planck - UBC Centre for Quantum Materials' at the University of British Columbia

Since 2013 Member of the board of directors of the 'Max Planck - EPFL Center for Molecular Nanoscience & Technology' at the École Polytechnique Fédérale de Lausanne (EPFL)

### Honors and Awards (Selection)

Since 1989 Honorary Professor for Theoretical Physics, TU Berlin

1998 Fellow of The American Physical Society

Since 2001 Honorary Professor for Theoretical Physics, FU Berlin

2001 Max Planck Research Award, jointly awarded by the Alexander von Humboldt Foundation and the MPG

2002 Ordinary Member of the Berlin-Brandenburgische Akademie der Wissenschaften

2003 Medard W. Welch Medal and Prize, awarded by the AVS, The Science & Technology Society

2004 Max-Born-Medal and Prize, jointly awarded by IOP (GB) and the DPG

2004-2012 'Visiting Professor' at the Dalian Institute of Chemical Physics of the Chinese Academy of Sciences

2007 Honorary doctorate, Faculty of Science at Lunds University, Sweden

2008 Ernst Mach Honorary Medal for Merit in the Physical Sciences, Academy of Sciences of the Czech Republic

2010 Rudolf Jaekel Prize of the German Vacuum Society (DVG)

### Cooperative Research Activities (since 2008)

Different projects with DFG, DAAD, BMBF, MPG, EU, ESF, NSF (USA), UCSB (USA), ARC (Australia), NSFC (China)

Invited or plenary speaker at 80 International Conferences during the past five years.

### Synergistic Activities (Conference Organization, Editorships, Advisory Boards)

Organizer and co-organizer of numerous conferences, workshops, summer schools (about 5 per year).

Member of various editorial boards, active in the DPG and APS on various levels.

Member of the CECAM council, member of the board of directors of the node [cecarn-mm1p.de](http://cecarn-mm1p.de).

Member of the board of trustees of psi-k.org.

Member of the scientific advisory board of the SUNCAT (Sustainable eEnergy through CA-Talysis) Center for Interface Science and Catalysis, Stanford, California.

Member of the advisory board of the "Materials Project Center for Functional Electronic Materials Design (DOE)" at Lawrence Berkeley National Laboratory.

Member of the Center for Nanophase Materials Sciences (CNMS) advisory committee at Oak Ridge National Laboratory (DOE), Oak Ridge.

Member of the advisory board of COMET “Computational Materials Education and Training” at Lawrence Berkeley National Laboratory.

Project coordinator of the Novel Materials Discovery (NOMAD) Center of Excellence, with 13 partners from 5 different countries, funded by the European Commission

Support of young researchers: 15 former members received professorships during the last 10 years

#### Publications

- 523 publications, total number of citations: 45.085, h-index = 117 (June, 2016, Google Scholar)

- Full publications list may be downloaded from: <http://th.fhi-berlin.mpg.de/site/index.php?n=Members.MatthiasScheffler>

## 2 Participant List

---

### Organizers

#### **De Vita Alessandro**

King's College London and University of Trieste

#### **Rubio Angel**

Max Planck Institute for the Structure and Dynamics of Matter

#### **Scheffler Matthias**

Fritz Haber Institute of the Max Planck Society (FHI), Berlin

#### **Blochwitz-Nimoth Jan**

Novalde, Germany

*Contacted*

#### **Bono Jose**

ISFOC, Spain

*Contacted*

#### **Braun Sylvie**

COMETFRI USA, Inc.

*Contacted*

#### **Constance John**

Novalde, Germany

*Contacted*

#### **Csany Gabor**

University of Cambridge, UK

*Positive response received*

#### **De Miguel Yolanda**

Tecnalia, Spain

*Contacted*



**del Caño Teodosio**

ONYX SOLAR ENERGY, S.L., Spain

*Contacted*

**Draxl Claudia**

Humboldt-Universität zu Berlin, Germany

*Positive response received*

**Ebner Reinhold**

Materials Center Leoben Forschung GmbH, Austria

*Contacted*

**Fernandez-Hevia Daniel**

INAEL Electrical Systems, S.A., Spain

*Contacted*

**Filip Sorin**

BP, UK

*Not contacted*

**Foster Adam**

Aalto University, Finland

*Positive response received*

**Ghiringhelli Luca**

Fritz-Haber-Institut der MPG, Germany

*Positive response received*

**Glawe Henning**

Max Planck Institute for the Structure and Dynamics of Matter, Germany

*Positive response received*

**Goddin James R.**

GRANTA, UK

*Contacted*

**Heinzel Stefan**

Max Planck Computing and Data Facility, Germany

*Positive response received*

**Helm Dirk**

Fraunhofer-Institut für Werkstoffmechanik, Germany

*Contacted*

**Hernandez Ruben Garcia**

Leibniz Supercomputing Centre, Germany

*Positive response received*

**Herrlinger Rolf**

Max Planck Innovation, Germany

*Contacted*

**Himanen Lauri**

Aalto University, Finland

*Positive response received*

**Huhs Georg**

Barcelona Supercomputing Center, Spain

*Positive response received*

**Ignatius Janne**

CSC – IT Center for Science Espoo, Finland

*Positive response received*

**Illas Francesc**

University of Barcelona, Spain

*Positive response received*

**Jurscha Helen**

Humboldt-Universität zu Berlin, Germany

*Positive response received*

**Kariyaa Ankit**

Fritz-Haber-Institut der MPG, Germany

*Positive response received*

**Kivioja Jani**

Nokia, Finland

*Positive response received*

**Klinge Michael**

Springer Materials, Germany

*Contacted*

**Koski Kimmo**

CSC – IT Center for Science Espoo, Finland

*Positive response received*

**Krein Michael**

Lockheed Martin, USA

*Contacted*

**Lampenscherf Stefan**

Siemens, Germany

*Contacted*

**Larsen Ask Hjorth**

Max Planck Institute for the Structure and Dynamics of Matter, Germany

*Positive response received*

**Lederer Hermann**

Max Planck Computing and Data Facility, Germany

*Positive response received*

**Levchenko Sergey**

Fritz-Haber-Institut der MPG, Germany

*Positive response received*

**Lushtinets Regina**

Novald, Germany

*Contacted*

**Martinez Cid Pedro Maria**

Iberdrola, S.A., Spain

*Contacted*

**McKane Angela**

BP Chemicals Limited, UK

*Contacted*

**Milman Victor**

Dassault Systemes BIOVIA, UK

*Contacted*

**Mohamed Fawzi**

Fritz-Haber-Institut der MPG, Germany

*Positive response received*

**Morreale Antonio**

Repsol, Spain

*Contacted*

**Moses Poul Georg**

Haldor Topsoe A/S, Danmark

*Contacted*

**Nieminen Risto**

Aalto University, Finland

*Positive response received*

**O'Brien Kylie**

Pintail Ltd., UK

*Positive response received*

**Pachter Pachter**

USAF, USA

*Not contacted*

**Pavone Pasquale**

Humboldt-Universität zu Berlin, Germany

*Positive response received*

**Perharz Gerhard**

Joanneum, Austria

*Contacted*

**Poelking Carl**

University of Cambridge, UK

*Contacted*

**Rampp Markus**

Max Planck Computing and Data Facility, Germany

*Contacted*

**Rieger Michael**

BASF, Germany

*Contacted*

**Riello Massimo**

General Electrics

*Not contacted*

**Rinke Patrick**

Aalto University, Finland

*Positive response received*

**Rupp Matthias**

Fritz-Haber-Institut der MPG, Germany

*Positive response received*

**Sanyal Suchismta**

Shell, India

*Contacted*

**Schaefer Angsar**

BASF SE, Germany

*Contacted*

**Schmitz Hardy R**

WISTA-MANAGEMENT GMBH, Germany

*Contacted*

**Sichirolo Antonio**

Greenetica GmbH, Austria

*Contacted*

**Sillanpää Atte**

CSC – IT Center for Science Espoo, Finland

*Positive response received*

**Spitaler Juergen**

Materials Center Leoben Forschung GmbH, Austria

*Contacted*

**Stella Martina**

King's College London, UK

*Positive response received*

**Stokbro Kurt**

Quantum Wise, Danmark

*Contacted*

**Strange Mikkel**

Technical University of Denmark

*Positive response received*

**Thygesen Kristian**

Technical University of Denmark

*Positive response received*

**Urban Daniel**

Fraunhofer-Institut für Werkstoffmechanik, Germany

*Contacted*

**Urreta Javier**

Tecnalia, Spain

*Contacted*

**Valero Rosendo**

University of Barcelona, Spain

*Positive response received*

**Wimmer Erich**

Materials Design, USA

*Contacted*

**Ziletti Angelo**

Fritz-Haber-Institut der MPG, Germany

*Positive response received*

**Zuliani Filippo**

Tata Steel, India

*Contacted*

## 3 Financial support

---

### Supports

**Funds requested from CECAM HQ : 4000€**

### Financial remarks

Accommodation (60 Euro for 1 night, 60 participants): 3600,- Euro, Dinner (40 Euro, 60 participants): 2400,- Euro  
-> Local costs: 6.000,- Euro

We plan to support the travel of 20 representatives from industry with 350 Euro -> Travel support: 7.000,- Euro

Total costs: 13.000,- Euro + travel costs for NOMAD associates.

We are very thankful that CECAM promised to support NOMAD workshops in a letter of support for NOMAD (October 2014). The NOMAD CoE is covering the bulk of the costs and we request a partial support of 4000 Euro from CECAM.

## 4 Suggested referees by Organizers

---