Psi-k Science Meeting Proposal Application Form for 2017 Events

Event Title:

Frontiers of Electronic-Structure Theory:
New Concepts and Developments in Density Functional Theory and Beyond

Symposium at the DPG (German Physics Society) Spring Meeting

Primary contact name	Matthias Scheffler
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Location of meeting	Dresden
Dates of meeting	Mar 19, 2017 - Mar 24, 2017
Proposed budget (€'s)	0,- We only ask for psi-k endorsement

Organizers:
John P. Perdew
Temple University, Philadelphia, Pennsylvania, USA
Angel Rubio
Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
Matthias Scheffler
Fritz Haber Institute of the Max Planck Society (FHI), Berlin, Germany

1. Scientific summary and Abstract

Abstract
Density functional theory (DFT) has made an unmatched contribution on providing first-principles atomistic insights to chemistry, condensed matter physics, materials science, and many other fields. The symposium will cover the recent progress in DFT by inviting well-known international experts as well as young researchers who have already significantly contributed to the field.

Scientific Summary
Most commonly used density functional approximations (DFAs) suffer from some well-known failures, including the incapability to correctly describe charge transfer processes, weak dispersion interactions, and strongly interacting scenarios. Recent effort attempting to cover such intricate many-body effects in DFT has initiated many new concepts at varying theoretical levels, and has led to a bunch of new concepts and insights, as well as new DFAs. Some of these developments can be viewed as a merger of wavefunction theories of quantum chemistry and DFT.

We expect this symposium to attract a diverse audience: those involved in method developments, practical DFT practitioners, as well as theoreticians in wave-function

theory, quantum Monte Carlo, GW, and other fields. A list of proposed topics for the invited speakers can be found in Section 1.3.

The symposium will be part of the DPG spring meeting 2017 in Dresden. With more than 7,000 expected participants the DPG spring meeting is the largest European physics conference (the second largest physics conference worldwide) covering all aspects of condensed matter and chemical physics, materials science, surface science, as well as polymer and biophysics, and more. For a few years now the conference language has been English.

This is an official symposium at the DPG spring meeting, which is hosted by the surface science division, but topics are not restricted to surface science. Everybody in the wider field of computational materials and electronic structure theory will be invited to attend and to submit an abstract.

2. Meeting Programme

We expect the Symposium to feature around 5 sessions from Tuesday to Thursday, which are usually comprised of one invited and app. 10 contributed talks. On Friday there will be a session with 5 invited talks. Invited talks last 30 minutes (25 minutes+5 minutes discussion) and contributed talks 15 minutes (12 minutes+3 minutes discussion). You can find the list of invited speakers in section 4.

3. Curriculum Vitae of Scientific Organiser including list of five most relevant

John P. Perdew
Laura H. Carnell Professor of Physics and Chemistry, Departments of Physics and Chemistry, College of Science and Technology, Temple University, Philadelphia, PA 19122, USA Homepage: https://phys.cst.temple.edu/john-perdew.html

Major Research Areas:
Density functional theory of electronic structure. Theory of molecules and materials.

Scientific Curriculum
1971 Ph.D. Cornell University - Physics
1971-74 Postdoctoral Fellow, University of Toronto
1974-77 Postdoctoral Fellow, Rutgers University
1977-79 Assistant Professor of Physics, Tulane University
1979-82 Associate Professor of Physics, Tulane University
1991-94 Department Chair, Tulane University
2001-03 Department Chair, Tulane University
1982-13 Professor of Physics, Tulane University
2013- Laura H. Carnell Professor of Physics and Chemistry, Departments of Physics and Chemistry, Temple University

Honors and Awards (Selection)
1990 LAS Award for Excellence in Research
1998 Work mentioned in the press release for the 1998 Nobel Prize in Chemistry awarded to Walter Kohn
2000 Tulane University Dissertation Director Award

2005 Provost's Research and Scholarly Achievement Award
2007 School of Science and Engineering First Annual Outstanding Researcher Award
2009 Perdew special issue, Journal of Chemical Theory and Computation
2011 Honorary Member, Tulane Alumni Association (one of 18)
2011 Election to the National Academy of Sciences (USA)
2012 Materials Theory Award, Materials Research Society
2015 Humboldt Reseach Award

Publications
- more than 250 publications, total number of citations: 176.461, h-index = 90 (June, 2016, Google Scholar)
- Full publications list may be downloaded from: https://phys.cst.temple.edu/~perdew/

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. Fisica 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

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 forScientific 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 Irradié, 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: "MaterialsEvolution", 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: 36of 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 studentsand 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-use ab initio computational materials research open-source project octopus (http://www.tddft.org). Itsimulates 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 fo 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 Eurepéen du Calcul Atomique et Moléculaire), Lausanne

(2015-) and of the Scientifc 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 inInformation Technology (ITAMIT), University of Minnesota, since 2003.
- External Advisory Board Member of The center for Nanotechnology and Molecular Materials, Wake Forest University, NorthCaroline, 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 Commision (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 isnow the Vicepresident for Scientific Development

Matthias Scheffler

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

Homepage: 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 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 Jaeckel Prize of the German Vacuum Society (DVG)
Since 2016	'Visiting Professor' at the Institute for Catalysis, Hokkaido University, Japan

Cooperative Research Activities (selection):

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.
- 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 cecam-mm1p.de.
- Member of the board of trustees of psi-k.org.
- Member of the advisory board of the "Materials Project Center for Functional Electronic Materials -Design (DOE)" at Lawrence Berkeley National Laboratory.
- Member of the advisory board of COMET "Computational Materials Education and Training" at Lawrence Berkeley National Laboratory.
- Member of the advisory board of CMI2 - Center for Materials Research by Information Integration of the National Institute for Materials Science in Japan.

- Member of the advisory board of the project "Development of Fundamental Technologies for Web-based Nano Science Platform" in Korea.
- Co-leader of the Max Planck Partner Group for Advanced Electronic-Structure Methods between University of Science and Technology of China and FHI, together with Xinguo Ren
- 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

4. Provisional list of proposed speakers/participants

Weitao Yang (Duke University, Durham, USA)
Andreas Savin (CNRS, Paris, France)
Igor Ying Zhang (Fritz Haber Institute, Berlin, Germany)
Kieron Burke (University of California, Irvine, USA)
Kristian S. Thygesen (Technical University of Denmark, Kongens Lyngby, Denmark)
Paola Gori-Giorgi (Universiteit Amsterdam, The Netherlands)
Arun Bansil (Northeastern University, Northeastern University, Boston, USA)
Neepa Maitra (Hunter College of the City University of New York, USA)

All listed speakers already agreed to participate

5. Primary Psi-k working group that the event relates to

Working group 1: Correlated electron systems