15TH ETSF YOUNG RESEARCHERS' MEETING (HAMBURG)



In 2018, the <u>ETSF Young Researchers' Meeting</u> took place in Hamburg, Germany. The hottest summer in the history of Hamburg, the well prepared Center for Free Electron Laser Science (CFEL) and more than sixty motivated researcher built the perfect frame for a stimulating week full of science.

The Young Researchers' Meeting (YRM) of the European Theoretical Spectroscopy Facility (ETSF) is an annual conference organized and attended exclusively by researchers without permanent position that work on state-of-the-art theoretical and computational methods for the study of electronic and optical properties of materials. YRM is the place to present your work in progress, come up with new ideas and learn about others' work in a friendly and open atmosphere. Master students, PhD students as well as young postdocs from all over Europe came together and discussed latest advances in their fields. This year, talks at the YRM were 20 minutes, including 5 minutes of discussion. This gave everyone enough time to communicate his or her

findings and receive feedback from other participants. The YRM started with a general introduction into the field of theoretical spectroscopy by Klaas Giesbertz, continued by five topical sessions plus poster, open, and an industry session, which will be depicted in more detail in following.

The five scientific sessions included:

- Old and new approaches towards material design. After an
 introduction with a focus on machine learning by Christopher A.
 Sutton, the participants talked about a variety of ab-initio methods to
 tackle the ground state electronic structure of novel materials.
- 2. **Theoretical spectroscopy.** Fabio Caruso started the session on spectroscopy by introducing the audience into optical spectroscopy methods. The approach of excited state structure closely connected to experimental settings made the main topic of this session.
- 3. Strongly correlated electrons, magnetism, and topological phases of matter. The session on correlated electrons started with a talk on quantum phases in condensed matter by Laura Fanfarillo. In the following, the participants discussed various correlation driven effects in solids.
- 4. **Fermion-boson systems in and out of equilibrium.** First, the participants received an introduction on fermion-boson interaction in solids by Denis Golež. Contributed talks with the main focus on electron-photon interaction continued this session. A second invited talk was given by Daniel Karlsson, who spoke about non-equilibrium Green's functions for coupled fermion-boson systems.
- 5. **Modelling properties of complex systems.** This session on larger scale reactions was introduced by Erik Hedegård, who spoke about a range of embedding theories and the embedding response theory in particular. Talks on structure prediction and molecular dynamics shaped the content of this session.

For a comprehensive list of scientific contributions from our ~60 participants, including the introduction lecture, the six keynotes, 37 contributed talks, and 16 posters, please see the website.

Traditionally, the YRM is not only a classical scientific conference with one talk after another, but it tries to explore also other opportunities of scientific exchange, social

interaction and interaction with the industry sector. This year, besides the traditional industry meeting, three new features were introduced: The introduction lecture, the scientific speed dating, and the open session.

On Monday, the conference started with a full 90 minutes introduction lecture by Klaas Giessbertz, in which he gave an overview over the main strategies to solve the many-body Schrödinger equation.

After the first session of scientific discussions, the day was finished with the scientific speed dating, where randomly chosen couples of participants had the chance to explain each other their area of research in very short time.

On Tuesday, we invited a panel of speakers from outside academia for the traditional industry session.

- Tim Baldsiefen from JenOptik explained us, what is important to switch between industry and academia and how interesting interdisciplinary work can become in industry
- Christoph Hübner and Malte Weinberg from the Otto Group told us, how even very abstract concepts from mathematics can be useful in everyday life with the example of artificial intelligence algorithms that they implemented for their company
- Sharon R. George, Swanand Marulkar, and Aratrika Roy from SpringerMaterials showed us their field of scientific work outside academia

We were especially delighted by SpringerMaterial's offer to organize an extra session about "Exploring pain points of researcher", where many participants joined.

After the industry session, we had the traditional poster session, accompanied by a delicious dinner, sponsored by Springer Materials.

On Wednesday, we had the honor to listen to the extraordinary and very diverse talks in the newly introduced "open session".

 Riku Tuovinen told us in his talk "Nonequilibrium Green's functions for dummies by a dummy" about the many details behind complicated numerical calculations and the many simple errors that he had to go through in achieving his results.

- César Rodríguez Rosario used the chance of the open session to explain us how
 thermodynamics and quantum mechanics can be combined. In his talk "How can
 Schrödinger's cat power a Carnot engine?" he condensed many research
 articles, which are the only source on this important topics as books and review
 articles on this field are missing so far, and hence provided us with an
 exceptional overview over the field.
- Markus Penz finished the open session in a striking talk with the title "Quasi-particles leave the lab," in which he used philosophic concepts to show that the boundaries between observer and observed object are much less fixed than we might have thought. He even extended these concepts to argue that physics is clearly "embedded in a net of technological, economical, and social agents. This refutes the romantic picture of science as a mirror on nature and in turn raises questions about responsibility and possible ways of conduct in natural sciences."

As in previous years, social programme was an important element of the conference to create opportunity for scientific and personal networking. The evening programme contained:

- The harbour tour on Monday, where the participants not only enjoyed spectacular views of one of Europe's largest harbours but also learned about its history as well as its environmental and socio-economic implications
- The social barbecue on Wednesday, which provided a nice break in the middle of exciting but tiring conference days. With good food and drinks as well as perfect weather, participants had the best opportunity to get to know one another!
- The beach volleyball tournament on Thursday, which was held on the ETSF YRM for the second time and which we hope will become a tradition

These activities allowed for a very friendly and collegial atmosphere throughout the entire week. It is the unique combination of state-of-the-art science and social networking what makes the YRM the perfect event for young scientist that are getting started the in the field. Therefore we are in particular happy that the YRM will continue next year for the 16th time in San Sebastian, Spain.

The ETSF YRM 2018 Organising Committee

Excerpts from the feedback form

- 100% found that keynotes were on an appropriate level
- Feedback on new features, introduced this year (people who gave at least 4 out of 5 possible points)

Introduction lecture: 82 %Scientific speed dating: 79 %

Open Session: 87 %

- Comments on the Open Session:
 - The open session was great.
 - The quality of all the talks in the open session was great!
 - Open session is a nice idea. Maybe we could have more(higher proportion) in the future.
 - Personally, I would not like it to be too philosophical. Discussion on our scientific thinking combined with historical overviews over certain fields are on the other hand, very welcome (IMO).
- General comments:
 - It was great!
 - Overall fantastic! The organisers were great; they dealt with every issue that arose extremely well which made for a smooth and pleasurable conference.
 - Really nice conference, very well organized, great people! Keep the Open Session! :-)
 - I must say that I enjoyed a lot this year's conference. The talks were really interesting and the organization was wonderful.
 - If you want more chemistry in invite chemists, but it should perhaps be more clear that most attendants are from a physics background.

Organising committee

- Florian Buchholz, PhD student, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
- Lars-Hendrik Frahm, PhD student, I. Institute for Theoretical Physics, University of Hamburg, Hamburg, Germany
- Uliana Mordovina, PhD student, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
- Christian Schäfer, PhD student, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Scientific Committee

- **Dr. Florian G. Eich**, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
- Dr. Johannes Flick, Harvard University, Boston, USA
- **Dr. Simone Latini**, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
- Dr. Nicolas Tancogne-Dejean, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
- **Dr. Riku Tuovinen**, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Supporting Organisers

- **Prof. Eberhard K. U. Groß**, Max Planck Institute of Microstructure Physics, Halle, Germany
- **Prof. Daniela Pfannkuche**, I. Institute for Theoretical Physics, University of Hamburg, Hamburg, Germany
- Dr. Lucia Reining, Irradiated Solids Laboratory, École Polytechnique, Palaiseau, France
- **Prof. Angel Rubio**, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
- Frauke Kleinwort, Administration, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
- **Gunda Sen**, Administration, I. Institute for Theoretical Physics, University of Hamburg, Hamburg, Germany

List of participants

- Abreu, Joao
- Bazzi, Sophia
- Berovic, Maja
- Biele, Robert
- Bröder, Jens

- Buchholz, Florian
- Bungey, Callum
- Caruso, Fabio
- Dangic, Djordje
- Delodovici, Francesco
- Entwistle, Mike
- Fanfarillo, Laura
- Ferradás, Rubén
- Giesbertz, Klaas
- Golez, Denis
- Guillaume, Le Breton
- Hampel, Alexander
- Hedegård, Erik
- Hirschmeier, Daniel
- Hodgson, Matt
- Hoffmann, Norah
- Hofmann, Damian
- Karlsson, Daniel
- Khalili, Khadijeh
- Kirwan, Amy
- Koskelo, Jaakko
- Krebs, Dietrich
- Laestadius, Andre
- Lorin, Arnaud
- Marques, Mário
- Mineo, Francesca
- Mohammed, Yusuf
- Monteiro Campos de Melo, Pedro Miguel
- Müller, Tristan
- O'Mahony, Shane
- Penz, Markus
- Peschke, Matthias
- Reinhard, Teresa,
- Reitz, Michael
- Rodríguez Álvarez, Matheus
- Rodríguez Rosario, César Alberto
- Rokaj, Vasil
- Singh, Nisha
- Steigemann, Conrad
- Suckert, Jens Renè
- Sun, Lin
- Sutton, Christopher
- Tchenkoue Djouom, Mary-Leena Martine

- Topp, Gabriel Elias
- Tuovinen, Riku
- Valencia, Ana M.
- Wang, Yanggang
- Wang, Chang-Ming
- Welakuh Mbangheku, Davis Dave
- Westergren, Jérémie
- Windgätter, Lukas
- Woehner, Kevin
- Yachmenev, Andrey
- Yang, Guang