Final Report ETSF YRM 2021

September 6-10, Cagliari (Italy)

The Young Researchers' Meeting (YRM) of the European Theoretical Spectroscopy Facility (ETSF) is an annual meeting which involves researchers in theoretical materials science at the early stages of their careers (i.e. PhD students and post-doctoral researchers).

ETSF YRM 2021 took place in Cagliari (Italy), in the frame of the wonderful and unique landscape of Sardinia. The conference has been held in the auditorium of the Faculty of Architecture, in the spectacular setting of Collegio dei Gesuiti, an historical building dating back to the 17th century. Because of the sanitary crisis due to Covid-19 pandemic, and because of the consequent necessity to maintain security distances, the number of participants was restricted. However, in order to give to all the applicants the possibility to attend the meeting, all the talks were broadcast via Zoom.

The YRM of ETSF aims to give to young researchers the opportunity to present their work and to share their knowledge in state-of-the-art theoretical methods for solid state physics, in an informal context which stimulates networking and exchange between peers. It also promotes meeting between young researchers and private companies interested in profiles with a strong scientific backgrounds. To this purpose, one of the session of the conference hosted some former researchers now working out of academia, which shared with the participants their experiences.

The meeting hosted five different sessions dealing with specific topics and approaches: the first session has been devoted to new methods in density-functional theory and Green's function-based methods aimed to tackle the problem of excited states; the second session focused on strongly correlated materials; in the third session we moved to vibrational properties and to their effect on the optical response of materials; during the fourth session we dealt with neutral excitations and optical properties of materials; finally, the fifth and last session was dedicated to multiscale modelling. Each session had one or two invited talks of the duration of 45 minutes each, plus 15 minutes for questions and discussion. Invited talks were followed by a series of contributed talks from the participants of 20 minutes (of which 15 for the presentation and 5 for questions). Finally also a poster session was held were the participants had also the chance to interact individually with the invited speakers.

Day 1

The conference started with the session dedicated to density-functional and Green's functions-based methods for excited-state properties. The session had two invited talks, the first one given by Nicola Colonna and titled "Spectral properties of molecules and solids from a functional approach". Here the speaker introduced density-functional theory pointing out advantages and limitations of the approach and giving a very nice overview of the current state-of-the-art methods to overcome such limitations, with a special regard for orbital-dependent approaches. A series of contributed talks mainly based on the GW method followed: "Frequency dependence in GW made simple using a multi-pole approximation" by Dario Leon, "Solving the Dyson equation via the algorithmic inversion" by Tommaso Chiarotti, "Higher-order many-body perturbation theory benchmarked on atoms" by Simone Vacondio, "First-principles electronic and structural properties of BNC nanomaterials" by Laura Caputo and "A GW study of dielectric screening effects on the quasiparticle properties of monolayer MoS2" by Nourdine Zibouche.

The afternoon was opened by the invited talk of Yaroslav Kvashnin on "Modelling magnetism

and strong correlations in real materials". The speaker gave a very pedagogical general introduction about the field of strongly correlated electron systems with a particular interest on magnetic properties, followed by a presentation of his original work. The session was continued with contributed talks from: Lorenzo Mariano on "A density-corrected DFT scheme applied to the calculation of spin-state energetics", Guido Falk von Rudorff on "Alchemical Perturbation Density Functional Theory: Scaling with chemical space", Ayoub Aouina on "New approximation to the exchange correlation potential from connector theory, application to the density of silicon and sodium chloride" and Gabriele Riva on "Photoemission spectroscopy from the three-body Green's function". At the end of the day most of the participants went to the beach close to Cagliari's city center as part of a social activity, where they took a swim and got to know each other over dinner and aperitifs.

Day 2

Tuesday has been devoted to vibrational properties of materials. The morning session has been opened by the invited talk of Konstanze Hahn, which gave an extremely pedagogical and clear presentation on the calculation of thermal conductivity using DFT. The invited talk has been followed by the contributions of R. Claes ("Phonon-limited carrier mobility in semiconductors from first principles"), A. El Sahili ("Perturbation theory beyond GW introduction to the GW-GWGWG approximation"), I. Maity ("Chiral valley phonons and flat phonon bands in moiré patterns of WSe2"), N. Rivano ("Polar optical phonons in one-dimensional materials") and K. Lively ("Simulating Vibronic Spectra without Born-Oppenheimer Surfaces").

In the afternoon the session moved towards the influence of phonons on the optical spectra of materials. The invited speaker Fulvio Paleari gave an extremely clear and interesting presentation on his pioneering work on the electron-exciton interaction. Several contributed talks followed, ranging from the role of phonons in the optical excitations in 2D systems (Francesco Libbi on "Phonon-assisted luminescence in defect centers from many body perturbation theory: the boron vacancy in 2D hBN", and Sara Postorino on "Direct and indirect excitons in monolayer and bilayer Molibdenum Ditelluride") to the influence of rare-earth doping on luminescence (J. Bouquiaux on "First-principle study of the luminescence spectrum of Eu2+, doped phosphors").

Day 3

Optical properties of materials were the focus of discussion on Wednesday. The morning session started with invited talk by Nicolas Tancogne-Dejean on "Advances in strong-field and ultrafast optical spectroscopies of solids". He discussed the standard optical spectroscopies and how they are usually modeled using ab initio methods. Then, he presented how novel experimental methods are simulated today and what are the remaining challenges posed by recent experimental advances. The invited talk has been followed by the contributions of Rajarshi Sinha-Roy on "Optical Magnetism in Nanoparticles from Real-Time TDDFT", Vitaly Gorelov on "Ab-initio investigation of electronic excitations in bulk V_2O_5", Lyudmyla Adamska on "Investigating dynamical Franz—Keldysh effects and beyond in bulk Germanium via TDDFT", Miki Bonacci on "Excitonic effects in graphene-like C_3N" and Pierre Lechifflart on "Optical properties of strained hexagonal Boron Nitride".

More contributed talks followed in the afternoon: Stefan Rost on "Electron energy loss spectroscopy (EELS) for 2D materials", Pedro Melo on "Optical properties of defect centers on 2D transition metal dichalcogenides", Kalyani Chordiya on "Real Time Observation of Correlated Electrons Response to Photo-Ionization", and Riccardo Reho on "Quasi-equilibrium states in heterobilayers of transition metal dichalcogenides". After the scientific talks, it took place the industry session, in which former researchers now working for private companies presented their professional transition and talked about job opportunities out of academia. This session included the contribution of Maja Berovic, former post-doctoral researcher and organiser of the previous ETSF YRM, now working as Data Analyst at LIST s.p.a (in Trieste), and Nicole Holzmann, formerly researcher in molecular dynamics and now working for Riverlane (in Oxford), a startup providing solutions for quantum computing.

Day 4

Thursday morning was dedicated to strongly correlated electron systems and relevant applications. The session was opened by the invited talk given by Anna Galler. She presented a recapitulating introduction to the physics of strong correlations, first introduced on Monday by Yaroslav Kvashnin. She discussed methods for going beyond single-site mean-field approximations, incorporating correlations on all length scales. She then gave a presentation on her recent work on rare-earth permanent magnets and correlated pigment materials. The rest of the morning continued with talks on different aspects of correlated systems.

During the afternoon the ceremony for the "Volker Heine Young Investigator Award 2021" was broadcast, in order to give the chance to all the participants to attend the talks from the five finalists: Bingqing Cheng on "Predicting material properties with the help of machine learning", Johannes Flick on "Strong light-matter coupling in molecular and extended systems from first principles", Federico Grasselli on "Invariance principles and topology in the ab initio charge transport of ionic fluids", Lionel Lacombe on "The exact factorization approach: From strongly correlated electrons to polaritonic chemistry", and Tianyu Zhu on "Full Cell Quantum Embedding for Correlated Materials".

In the evening the social dinner took place in a nice pizzeria in the historical center of Cagliari, where all the participants had the chance to interact in a less formal environment.

Day 5

The fifth day of the conference (including a program only for the morning) marked the end of the Young Researchers' Meeting 2021. It started with an invited talk given by Bingqing Cheng who introduced the session on multiscale modelling. She also discussed recent work of hers on exploiting machine-learning methods to extend the scope of atomistic simulations. The morning continued with the contributed talks from Loris Ercole on "Doping solid-state electrolytes: a pinball model study", Massimiliano Comin on "Embedded many-body petrubation theory for complex molecular systems: fundamentals and applications to doped semiconducting polymers", Pierre-Paul De Breuck on "Materials property prediction for limited datasets and bias-imbalance in data-driven materials

science" and Thomas Baker on "Lanczos recursion on a quantum computer for the Green's function and wavefunctions."

Before closing the conference the two best posters selected by the participants and by the invited speakers were announced and the winners rewarded with a scientific book of their choice.

Best posters

The best poster award chosen by the invited speakers and the participants was given to:

- Alam Osorio, for the poster titled "Towards the electronic density response of borophene polymorphs";
- Jörn Stöhler, for the poster titled "Implementation of the Bethe-Salpeter equation in the SPEX code".

Participants' survey

In the following we report the results of the survey filled out by the participants. More than 80% of the participants completed the form so the results below provide a good overview of the outcome of the conference. Votes go from 1 (very bad) to 5 (very good).

	1 Very bad	2 Bad	3 Ok	4 Good	5 Very good	Average
How would you rate the ETSF YRM 2021 overall?	-	-	-	20.5%	79.5%	**4.8**
How well organized do you feel the conference was?	-	-	5.1%	30.8%	64.1%	**4.6**
How did you find the talks from the invited speakers?	-	-	-	51.3%	48.7%	**4.5**
How did you find the organization of the daily timetable?	-	-	7.7%	38.5%	53.8%	**4.5**
How did you find the poster session?	-	-	17.9%	43.6%	38.5%	**4.2**
How did you find the industry session?	-	5.1%	35.9%	46.2%	12.8%	**3.7**
How did you find the choice of Cagliari as the conference location?	-	-	2.6%	15.4%	82.0%	**4.8**

How did you find the auditorium and outside space of the conference?	-	-	10.3%	28.2%	71.8%	**4.8**
How did you find the atmosphere between the conference participants?	-	-	2.6%	25.6%	71.8%	**4.7**
How would you rate communication with the organizing committee?	-	-	-	25.6%	74.4%	**4.7**
Considering the low conference fee, how did you find the coffee breaks?	-	-	10.2%	15.4%	74.4%	**4.6**
Considering the low conference fee, how did you find the lunch breaks?	-	5.1%	25.7%	41.0%	28.2%	**3.9**
Considering the low conference fee, how did you find the social dinner?	-	2.5%	15.4%	30.8%	51.3%	**4.3**
Considering the low conference fee, how did you find the accommodation?	-	2.9%	11.8%	58.8%	26.5%	**4.1**

In the following we also report some of the most relevant comments:

- *"It was an extraordinary great experience, meeting other young scientists in this great enviroment with enough time to connect"*
- *"Thank you for organizing the conference, it has been a very pleasant experience"*
- *"It could be better to prepare water for the poster session"*
- *"I found it a pity that there was no real social event organized at the beach, or organized visit of the city"*

Final impressions

The feedback from the participants was extremely positive, almost everyone was quite satisfied with the scientific level of the conference as well with the overall organization. Despite the difficulties due to the Covid-19 restrictions, the participants had the chance (the first in two years for most of them!) to meet, network and interact with each other, sharing their work with others and, even more importantly, building up connections. The main difficulties came from the desire of realizing a meeting in a hybrid format in order to give the chance to all the people interested to participate. Eventually setting up this kind of format was quite challenging and probably unnecessary (in normal times) given the low number of people who actually attended the conference from remote. Considering also that one of the main purposes of this meeting remains that of realizing a network between young researchers, we suggest future organizers to opt for a meeting fully in presence.

The website will keep reachable at the following link:
https://sites.google.com/view/etsfyrm2021