



## MaX School on Advanced Materials and Molecular Modelling with Quantum ESPRESSO | (SMR 3622)

17 May 2021 - 28 May 2021  
Virtual, Italy

### 6 Directors

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1. <b>BARONI Stefano</b>	SISSA	Italy
2. <b>GEBAUER Ralph</b>	ICTP	Italy
3. <b>GIROTTI Ivan</b>	ICTP	Italy
4. <b>KOKALJ Anton</b>	Jožef Stefan Institute	Slovenia
5. <b>REN Wei</b>	Shanghai University	People's Republic of China
6. <b>STROPPA Alessandro</b>	CNR-SPIN	Italy

### 9 Lecturers

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1. <b>BASEGGIO Oscar</b>	SISSA	Italy
2. <b>BERCX Marnik</b>	EPFL	Switzerland
3. <b>BONFÀ Pietro</b>	University of Parma	Italy
4. <b>DE GIRONCOLI Stefano Maria</b>	Sissa	Italy
5. <b>DELUGAS Pietro Davide</b>	SISSA	Italy
6. <b>GIANNOZZI Paolo</b>	Universita' di Udine Dipartimento di Scienze Matematiche, Informatiche e Fisiche	Italy
7. <b>SCANDOLO Sandro</b>	ICTP	Italy
8. <b>SEITSONEN Ari Paavo</b>	Ecole Normale Supérieure ENS, CNRS Département de Chimie	France
9. <b>TIMROV Iurii</b>	Ecole Polytechnique Fédérale de Lausanne (EPFL) EPFL STI IMX THEOS	Switzerland

### 7 Speakers

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1. <b>BLUEGEL Stefan Norbert</b>	Forschungszentrum Jülich GmbH Institut für Festkörperforschung	Germany
2. <b>CAR Roberto</b>	Princeton University Department of Chemistry	United States of America
3. <b>CARNIMEO Ivan</b>	SISSA	Italy
4. <b>GONG Xingao</b>	Fudan University	People's Republic of China
5. <b>MAURI Francesco Giovanni Maria</b>	University of Rome Sapienza	Italy

6.	<b>MOLINARI Elisa</b>	Max Centre of Excellence	-
7.	<b>SPALDIN Nicola Ann</b>	ETHZ	Switzerland

## 21 Tutors

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1.	<b>BERTOSSA Riccardo</b>	SISSA	Italy
2.	<b>CHANDRAMATHY SURENDRAN Praveen</b>	Cochin University of Science and technology International School of Photonics	Indonesia
3.	<b>CONTE Felice</b>	University of Naples Federico II, Department of Physics Ettore Pancini	Italy
4.	<b>CUI Yaning</b>	SHU EDU	People's Republic of China
5.	<b>DOS SANTOS Flaviano José</b>	EPFL	Switzerland
6.	<b>GHOSH Sukanya</b>	ICTP	Italy
7.	<b>HUŠ Matej</b>	National Institute of Chemistry Department of Catalysis and Chemical Reaction Engineering	Slovenia
8.	<b>JIANG Tao</b>	International center for quantum and molecular structures	People's Republic of China
9.	<b>MALICA Cristiano</b>	SISSA Condensed Matter Theory	Italy
10.	<b>MONDAL Unmesh</b>	Indian Institute of Science Education and Research Chemistry Department	India
11.	<b>PEGOLO Paolo</b>	SISSA	Italy
12.	<b>POBERZNIK Matic</b>	SISSA	-
13.	<b>QIAO Lei</b>	International Centre for Quantum and Molecular Structures, Shanghai University	People's Republic of China
14.	<b>RAMIREZ Francisco</b>	EPFL THEOS, STI	Switzerland
15.	<b>SAFARI Mandana</b>	SISSA, CM group	Italy
16.	<b>SAPPATI Subrahmanyam</b>	Esearch Raman Institute	-
17.	<b>SEWELL Christopher</b>	EPFL	Switzerland
18.	<b>STAVRIC Srdan</b>	University of Trieste Physics Department	Italy
19.	<b>TISI Davide</b>	SISSA	Italy
20.	<b>URRU Andrea</b>	ETH	Swaziland
21.	<b>VELANKANNI Nandhakumar</b>	The Abdus Salam International Centre for Theoretical Physics	Italy

## 107 Participants

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1.	<b>AGBAOYE Ridwan Olamide</b>	Applied Science Department Federal College of Dental Technology and Therapy Enugu	Nigeria
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2.	<b>AHN Yunho</b>	Commissariat à l'énergie atomique et aux énergies alternatives	France
3.	<b>ALAA MOHAMMED IDRIS BAKHIT -</b>	EAI FR	Rwanda
4.	<b>ALDARAWSHEH Amal Jawdat Nayef</b>	University of Duisburg-Essen	Germany
5.	<b>ALLIATI Ignacio Martin</b>	Queen's University Belfast ASC	United Kingdom
6.	<b>ALVES PACHECO MOREIRA Ricardo Manuel</b>	Universidade do Porto IFIMUP	Portugal
7.	<b>BABARIYA Bindiya Sanjaybhai</b>	Gujarat University Department of Physics	India
8.	<b>BENZIDI Hind</b>	Institut FOTON Site INSA Rennes	France
9.	<b>BHARDWAJ Sunayana</b>	Jawaharlal Nehru University New Delhi Phd in Nanoscience under Prof. Bijoy kumar Kuanr, Special centre for Nanoscience (SCNS)	India
10.	<b>BIJELIC Lazar</b>	-	Serbia
11.	<b>BODESHEIM David Manuel</b>	Technical University of Dresden Faculty of Mechanical Science and Engineering	Germany
12.	<b>BÖGELS Timoteüs Franciscus Johannes</b>	École Normale Supérieure de Lyon Laboratoire de Géologie de Lyon	France
13.	<b>BORGHESI Costanza</b>	-	Italy
14.	<b>BOUKACHABIA Samira</b>	Badji Mokhtar Annaba University Department of Physics	Algeria
15.	<b>BRAVETTI Federica</b>	University of Torino Department of Chemistry	Italy
16.	<b>BUTA Maria-Cristina</b>	Institute of Physical Chemistry "I. Murgulescu" Theoretical and Structural Chemistry Laboratory	Romania
17.	<b>BYARUHANGA Paul</b>	Makerere University Department of Physics	Uganda
18.	<b>CALDARELLI Giovanni</b>	University of Rome "La Sapienza", Department of physics	Italy
19.	<b>CARTA Alberto</b>	ETH Zurich D-MATL	Switzerland
20.	<b>CHENG Xiyue</b>	Chinese Academy of Sciences Fujian Institute of Research on the Structure of Matter	People's Republic of China
21.	<b>CHEVALLIER-BOUTELL Ignacio José</b>	Universidad Nacional de Córdoba Facultad de Matemática, Astronomía y Física	Argentina
22.	<b>DE BARROS BARBOSA Maria Carolina</b>	Faculdade de Ciências da Universidade do Porto Departamento de Física e Astronomia	Portugal
23.	<b>DE MATOS LAMELAS Afonso Xavier</b>	Physics Department of the University of Aveiro	Portugal
24.	<b>DEY Urmimala</b>	Indian Institute of Technology Kharagpur	India
25.	<b>DOS SANTOS CASTRO Giselle</b>	Universidade Federal do Ceará	Brazil

26.	<b>DUAN Xiang-Mei</b>	Faculty of Science, Department of Physics, Ningbo University,	People's Republic of China
27.	<b>DUDDY Ryan Joseph</b>	Queen's University Belfast	United Kingdom
28.	<b>ESTERAS CORDOBA Dorye Luis</b>	Instituto de Ciencia Molecular	Spain
29.	<b>GAHUTU RUGWIRO Elysee</b>	University of Rwanda Department of physics	Rwanda
30.	<b>GAJERA Udaykumar Hiralal</b>	Consiglio Nazionale delle Ricerche SuPerconducting and other INnovative materials and devices institute	Italy
31.	<b>GREGORI Erik</b>	University of Ljubljana FKKT, UniLJ, SI	Slovenia
32.	<b>GUO Qilin</b>	ICQMS Shanghai University	People's Republic of China
33.	<b>HABAMAHOBO Thacien</b>	University of Rwanda Department of Physics	Rwanda
34.	<b>HAGUMIMANA Jean Paul</b>	University of Rwanda Department of Physics	Rwanda
35.	<b>HAMLAT Mama</b>	University of Saida Department of Physics	Algeria
36.	<b>HANIŠ Jozef</b>	Pavol Jozef Šafárik University, Košice Department of Theoretical Physics and Astrophysics	Slovak Republic
37.	<b>HERNANDEZ BERTRAN Michael Alejandro</b>	UNIMORE Dipartimento di Scienze Fisiche, "FIM"	Italy
38.	<b>HO Viet Thang</b>	Da Nang University of Science and Technology Department of Chemical Engineering	Viet Nam
39.	<b>HUNANYAN Areg</b>	Yerevan State University	Armenia
40.	<b>INIS DEMIR Gozde</b>	Istanbul Technical University Computational Science and Engineering Programme	Turkey
41.	<b>JIMÉNEZ DÍAZ Laura Michelle</b>	Universidad Nacional Autónoma de México Faculty of Chemistry	Mexico
42.	<b>JIN Yichen</b>	Shanghai University Department of Physics	People's Republic of China
43.	<b>JOHNSON E Jessica</b>	Jessica Johnson, Graduate Research Assistant, Materials Science and Engineering Department, Rutgers University	United States of America
44.	<b>JURECZKO Paulina Zuzanna</b>	Institute of Physics	Poland
45.	<b>KETY Kossi</b>	EAI FR	Rwanda
46.	<b>KHOSRAVI Ali</b>	SISSA, International School for Advanced Studies ICTP, The Abdus Salam International Centre for Theoretical Physics	Italy
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48.	<b>KULHARI Neeraj</b>	IIS (Deemed to be University), Jaipur, Rajasthan, India	India

49.	<b>LEVIN ROJAS Natalia</b>	Max Planck Institute for Chemical Energy Conversion Department of Molecular Catalysis	Germany
50.	<b>LIN Changpeng</b>	École Polytechnique Fédérale de Lausanne Theory and Simulation of Materials	Switzerland
51.	<b>LONCARIC Ivor</b>	Rudjer Boskovic Institute Division of Theoretical Physics	Croatia
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56.	<b>MENG'WA Victor Kirui</b>	Alupe University College Department of Physics and Computer Science	Kenya
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60.	<b>NAGY Gergely Norbert</b>	ELI-ALPS	Hungary
61.	<b>NEVES CESÁRIO António Duarte</b>	FCUP IFIMUP	Portugal
62.	<b>NGOIPALA Apinya</b>	University of Limerick Department of Chemical Sciences	Ireland
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68.	<b>OGENYI Sunday Joseph</b>	-	Nigeria
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82.	<b>RODRÍGUEZ LOSADA María</b>	University of Granada Department of Atomic, Molecular and Nuclear Physics	Spain
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100.	<b>TRANDAFIR Anamaria</b>	University of Bath Department of Physics	United Kingdom
101.	<b>UMM-E-HANI -</b>	Jacob University Bremen Department of Physics and Earth Sciences	Germany
102.	<b>ÜNSAL Elif</b>	-	Turkey
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107.	<b>ZULLO Ludovica</b>	-	Italy