

Monday 23 June

Session A1 – 8:30	Session B1	Session C1	Session D1	Session E1	
CATALYSIS & REACTIVITY	ELECTRONIC-STRUCTURE THEORY	BIOSYSTEMS	COMPUTING & SOFTWARE	CHEMICAL STRUCTURE & BONDING	
Reactants, reactions, and catalysis	Green's function methods	Cheminformatics & medicinal chemistry	Quantum computing	Conjugated systems	
Kevin Naidoo	Andreas Görling	Stacey Wetmore	Ivan Kassal	Peter Schreiner	
Raghavan Sunoj	963 Dominika Zgid	924 Jean-Louis Reymond	986 Birgitta Whaley	919 Debashree Ghosh	871
Stuart Macgregor	926 Wim Klopper	458 Jan Řezáč	480 Artur Izmaylov	131 Abhik Ghosh	973
Ashique Lal	207 Marios-Petros Kitsaras	124 Elfi Kraka	130 Davide Castaldo	327 Martin Rahm	23
Boris Maryasin	127 Arno Förster	572 Jean-Philip Piquemal	699 Karl Michael Ziems	260 Takafumi Shiraogawa	313
Session A2 - 10:20	Session B2	Session C2	Session D2	Session E2	
MACHINE LEARNING	CATALYSIS & REACTIVITY	ELECTRONIC-STRUCTURE THEORY	BIOSYSTEMS	ELECTRONIC-STRUCTURE THEORY	
ML for simulations	Surfaces and heterogenous catalysis	Numerical methods and techniques	Macromolecules	Ultrahigh accuracy and QED	
Heather Kulik	Angel Martín Pendás	Stefan Grimme	Benedetta Mennucci	Fritz Schaefer	
Gábor Csányi	967 Philippe Sautet	873 Peter Gill	953 Lynn Kamerlin	49 Trond Saue	349
Alexandre Tkatchenko	995 Núria López	972 Luca Frediani	896 Subha Kalyaanamoorthy	653 Jacek Komasa	178
Jelle Vekeman	785 Christopher Stein	287 Alexander Stark	157 Xiang Sheng	196 Ádám Margócsy	775
Michael Gillhofer	317 Mireia Segado-Centellas	716 Eduard Matito	136 Adil Kabylda	547 Pekka Pyykkö	486
Session A3 – 13:20	Session B3	Session C3	Session D3	Session E3	
ELECTRONIC-STRUCTURE THEORY	ENERGY & MATERIALS	CATALYSIS & REACTIVITY	QUANTUM DYNAMICS	BIOSYSTEMS	
Coupled-cluster theory	Condensed systems	Molecular and reaction design	Nonadiabatic dynamics	Macromolecules	
Jürgen Gauss	Yi Qin Gao	Vidar Remi Jensen	Ove Christiansen	Elfi Kraka	
Piotr Piecuch	923 Francesco Paesani	752 Yousung Jung	441 Alicia Palacios	804 Ferran Feixas	622
Henrik Koch	862 Damien Laage	918 Jan H. Jensen	440 Jian Liu	86 Taye Demissie	673
Karol Kowalski	199 Jochen Blumberger	54 Kevin Naidoo	171 Peter Schürger	166 Petra Imhof	339
Francesco Evangelista	348 Marco Nascimento	223 Gyula Hoffka	815 Oliver Kühn	412 Ana Gamiz-Hernandez	917
Session A4 – 15:10	Session B4	Session C4	Session D4	Session E4	
ELECTRONIC-STRUCTURE THEORY	MACHINE LEARNING	BIOSYSTEMS	CHEMICAL STRUCTURE & BONDING	QUANTUM DYNAMICS	
Explicit correlation	ML for chemical reactions	Macromolecules	Early elements	Ultrafast dynamics	
Wim Klopper	Sigbjørn Løland Bore	Qiang Cui	Gabriel Merino	Thomas Bondo Pedersen	
Seiichiro Ten-no	874 Boris Kozinsky	971 Modesto Orozco	819 Miroslav Urban	270 Françoise Remacle	887
Ali Alavi	853 Fernanda Duarte	842 Alessandra Magistrato	202 ED Jemmis	163 Michal Repisky	962
Éva Zsuzsanna Mihálka	470 Joakim Jestilä	246 Mariastella Cascone	544 Celina Sikorska	738 H. Bernhard Schlegel	197
Silvia di Grande	587 Jessica White	667 David Carrasco De Busturia	165 Tatiana Korona	276 Jonathan Fetherolf	701
Session A5 – 17:00	Session B5	Session C5	Session D5	Session E5	
ELECTRONIC-STRUCTURE THEORY	MACHINE LEARNING	COMPUTING & SOFTWARE	QUANTUM DYNAMICS	CATALYSIS & REACTIVITY	
Density-functional development	ML for chemical design	Quantum computing	Ultrafast dynamics	Electrochemistry and related	
Weitao Yang	David Balcells	Birgitta Whaley	Federica Agostini	Cristina Trujillo	
Martin Head-Gordon	957 Clémence Corminbœuf	446 Ivan Kassal	356 Fernando Martín García	663 Samira Siahrostami	21
Erin Johnson	505 Anatole von Lilienfeld	442 Marco Govoni	1007 Ove Christiansen	959 Maria Besora	402
Fritz Schaefer	687 Konstantinos Vogiatzis	10 Maria-Andreea Filip	419 Jiří Vaniček	691 Tangui Le Bahers	169
Viktor Staroverov	154 Thijs Stuyver	43 Yu Zhang	20 Nazanin Jamshidi	140 Melissa Manetsch	362

Tuesday 24 June

Session A1 – 8:30	Session B1	Session C1	Session D1	Session E1	
CATALYSIS & REACTIVITY	ELECTRONIC-STRUCTURE THEORY	BIOSYSTEMS	ELECTRONIC-STRUCTURE THEORY	SPECTROSCOPY	
Surfaces and heterogenous catalysis	Many-body methods & NC1	Bio/nanosystems	Relativistic quantum chemistry	Polarization models	
<i>Stuart Macgregor</i>	<i>Seiichiro Ten-no</i>	<i>Michele Cascella</i>	<i>Trond Saue</i>	<i>Russell Boyd</i>	
Anastassia Alexandrova	38 Katarzyna Pernal	875 Daan Frenkel	703 Wenjian Liu	436 Benjamin Stamm	798
Ataulpa Braga	901 Janus Juul Eriksen	810 Wataru Shinoda	782 Jürgen Gauss	438 Kaline Coutinho	938
Mikhail Polynski	357 Daniel Boese	443 Katie Wilson	97 Achintya Kumar Dutta	215 Cedrix Dongmo Fomthui	624
Basil Raju	47 Andreas Hansen	121 João Coimbra	597 Erik Donovan Hedegård	497 Tommaso Nottoli	305
Session A2 – 10:20	Session B2	Session C2	Session D2	Session E2	
CATALYSIS & REACTIVITY	ENERGY & MATERIALS	ELECTRONIC-STRUCTURE THEORY	QUANTUM DYNAMICS	BIOSYSTEMS	
Molecular and reaction design	Materials and energy	Berry phase & complex wave functions	Ultrafast dynamics	Bio/nanosystems	
<i>Odile Eisenstein</i>	<i>Leticia González</i>	<i>Henrik Koch</i>	<i>Fernando Martín García</i>	<i>Modesto Orozco</i>	
Satoshi Maeda	307 Laura Gagliardi	702 Hardy Gross	949 Federica Agostini	388 Biswarup Pathak	921
Markus Reiher	80 Elena Besley	763 Joseph Subotnik	686 Morgane Vacher	820 Matteo Dal Peraro	728
Derek Ahneman	161 Tim Kowalczyk	239 Ansgar Pausch	581 Yi Zhao	720 Gioacchino Schifino	580
Giovannimaria Piccini	698 Shubhajt Das	609 Bang Huynh	191 Angela Wilson	680 Samaneh Davoudi	79
Session A3 – 13:20	Session B3	Session C3	Session D3	Session E3	
ELECTRONIC-STRUCTURE THEORY	MACHINE LEARNING	MOLECULAR DYNAMICS	QUANTUM DYNAMICS	CHEMICAL STRUCTURE & BONDING	
Density-functional development	ML for chemical reactions	Honorary session: 40 years of AIMD	DMRG and MCTDH	f-block elements	
<i>Miroslav Urban</i>	<i>Francesco Paesani</i>	<i>Matteo Dal Peraro</i>	<i>Françoise Remacle</i>	<i>Pekka Pyykkö</i>	
Kieron Burke	922 Teresa Head-Gordon	847 Roberto Car	987 Irene Burghardt	666 Karin Fink	722
Eunji Sim	807 Dennis Salahub	91 Ursula Röthlisberger	960 Zhigang Shuai	773 Miho Hatanaka	713
Jacques Desmarais	128 Jordi Buils	479 Mark Tuckerman	395 Yuki Kurashige	56 Sergey Varganov	524
Priya Priya	692 Haobo Li	26 Amin Alibakhshi	771 Henrik Larsson	134 Meagan Oakley	700
Session A4 – 15:10	Session B4	Session C4	Session D4	Session E4	
CATALYSIS & REACTIVITY	SPECTROSCOPY	BIOSYSTEMS	ELECTRONIC-STRUCTURE THEORY	ENERGY & MATERIALS	
Surfaces and heterogenous catalysis	Methods for excited electronic states	Multiscale modelling	Strong correlation & entanglement	Condensed systems	
<i>Philippe Sautet</i>	<i>Frank Neese</i>	<i>Marco De Vivo</i>	<i>Piotr Piecuch</i>	<i>Marco Nascimento</i>	
Annabella Selloni	748 Emmanuel Fromager	755 Benedetta Mennucci	832 Shuhua Li	881 Nicola Gaston	955
Akira Nakayama	681 Weitao Yang	956 Paula Homem-de-Mello	685 Mario Piris	16 Pavel Jungwirth	664
Seungjae Kwak	437 Momir Mališ	787 Yingjie Wang	117 Jiří Pittner	77 Sheh-Yi Sheu	19
Francesc Viñes Solana	89 Lars Goerigk	139 Sebastian Reiter	594 Sarai Dery Folkestad	94 Jun-Ho Choi	50
Session A5 – 17:00	Session B5	Session C5	Session D5	Session E5	
BIOSYSTEMS	ELECTRONIC-STRUCTURE THEORY	CATALYSIS & REACTIVITY	SPECTROSCOPY	EXOTIC SYSTEMS	
Cheminformatics & medicinal chemistry	Methods for larger systems	Reactants, reactions, and catalysis	Circular dichroism	Strong fields and high pressure	
<i>Ursula Röthlisberger</i>	<i>David Sherrill</i>	<i>Annia Galano</i>	<i>Kenneth Ruud</i>	<i>Peter Schwerdtfeger</i>	
William Jorgensen	808 Christian Ochsenfeld	952 David Wales	969 Daniel Crawford	757 Stella Stopkowicz	941
Zoe Cournia	981 Hiromi Nakai	723 Feliu Maseras	674 Luuk Visscher	814 Andrew Wibowo-Teale	671
Stacey Wetmore	321 Filippo Lipparini	826 Sebastian Kozuch	2 WanZhen Liang	243 Eva Zurek	697
Christoph Riplinger	714 Maristella Alessio	187 Masataka Nagaoka	44 Marco Caricato	138 Mercedes Alonso	393

Thursday 26 June

Session A1 – 8:30	Session B1	Session C1	Session D1	Session E1	
ELECTRONIC-STRUCTURE THEORY	SPECTROSCOPY	BIOSYSTEMS	CHEMICAL STRUCTURE & BONDING	ENERGY & MATERIALS	
Methods for periodic systems	Methods for excited states	Multiscale modelling	Analysis	Photophysics and photochemistry	
Christian Ochsenfeld	Emmanuel Fromager	Stefano Vanni	Henry Rzepa	Zhigang Shuai	
Georg Kresse	831 Julia Westermayr	364 Qiang Cui	689 Matthias Bickelhaupt	670 Dage Sundholm	797
Lin Lin	571 Hannes Jónsson	660 Garnet Chan	872 Frank de Proft	813 Jing Ma	888
David Tew	870 Thomas Froitzheim	81 Andrea Pérez-Villa	504 Inbal Tuvi-Arad	749 Dana Nachtigallová	636
Philip Hoggan	13 Elli Selenius	790 Andrea Levy	601 Jacob Toney	394 Sofia Canola	582
Session A2 - 10:20	Session B2	Session C2	Session D2	Session E2	
ELECTRONIC-STRUCTURE THEORY	CATALYSIS & REACTIVITY	BIOSYSTEMS	ENERGY & MATERIALS	COMPUTING & SOFTWARE	
Simpler model systems	Reactants, reactions, and catalysis	Multiscale modelling	Photophysics and photochemistry	Software	
Anna Krylov	Manuel Yañez	Garnet Chan	Dage Sundholm	Daniel Crawford	
Stefan Grimme	825 Evert Jan Meijer	943 Carme Rovira	863 Kumar Vanka	899 Patrick Norman	898
Peter Schwerdtfeger	92 Bastian Skjelstad	715 Marco De Vivo	817 Leticia González	964 Susi Lehtola	799
Per Siegbahn	212 Amalia Poblador Bahamonde	880 Stefano Serapian	120 Enrico Tapavicza	523 John Herbert	24
Itai Panas	679 Zhexuan Song	654 Allison Keys	226 Enrique Manuel Arpa	411 David Sherrill	513
Session A3 – 13:20	Session B3	Session C3	Session D3	Session E3	
ELECTRONIC-STRUCTURE THEORY	CATALYSIS & REACTIVITY	MACHINE LEARNING	SPECTROSCOPY	TEACHING & EDUCATION	
Density-functional development	Molecular and reaction design	ML for simulations	Rotovibrational spectra	Teaching & education	
Jiali Gao	Ainara Nova	Konstantinos Vogiatzis	Sonia Coriani	Trygve Helgaker	
Stefan Vučković	837 Annia Galano	508 Yi Luo	737 Attila Császár	931 Anders Mølthe-Sørenssen	998
Martin Kaupp	661 Vidar Remi Jensen	946 Yi Qin Gao	882 Guntram Rauhut	106 Peter Taylor	1001
Hans Jørgen Aa. Jensen	457 Cristina Trujillo	36 Amanda Arcidiacono	537 Ayaki Sunaga	735 Dirk Andrae	367
Aaron Garrison	159 Wataru Matsuoka	237 Krzysztof Szalewicz	730 Frederik Tielens	72 Henry Rzepa	12
Session A4 – 15:10	Session B4	Session C4	Session D4	Session E4	
CATALYSIS & REACTIVITY	ENERGY & MATERIALS	ELECTRONIC-STRUCTURE THEORY	MACHINE LEARNING	SPECTROSCOPY	
Reactants, reactions, and catalysis	Materials and energy	Optimization in quantum chemistry	ML for electronic structure	Positrons & weak interactions	
Feliu Maseras	Evert Jan Meijer	Erik Tellgren	Hiromi Nakai	Edit Mátyus	
Jin Wen	800 Debra Bernhardt	751 Éric Cances	742 Paola Gori-Giorgi	867 Gustavo Aucar	861
Fahmi Himo	928 Sara Bonella	827 Roland Lindh	672 Matthias Kick	233 Robert Berger	360
Johannes Hoja	575 Virginia Carnevali	538 Giovanni Scalmani	619 Angel Martín Pendás	58 Dermot Green	256
Michele Assante	769 Tuanan Lourenço	334 Hugh Burton	712 Tomáš Bučko	214 Kenneth Jordan	1
Session A5 – 17:00	Session B5	Session C5	Session D5	Session E5	
SPECTROSCOPY	ELECTRONIC-STRUCTURE THEORY	ENERGY & MATERIALS	BIOSYSTEMS	CHEMICAL STRUCTURE & BONDING	
Spectroscopy & energy surfaces	Beyond standard DFT	Materials and energy	Bio/nanosystems	Coordination chemistry	
Abriel Castro	Paola Gori-Giorgi	Laura Gagliardi	Carme Rovira	ED Jemmis	
Sonia Coriani	925 Paul Ayers	733 Marie-Liesse Doublet	966 Sergio Pantano	417 Gabriel Merino	392
Anna Krylov	382 Jiali Gao	904 Emi Minamitani	93 Cristiana Di Valentin	794 Jeanet Conrادية	118
Ida-Marie Høyvik	721 Andreas Görling	220 Gloria I. Cárdenas-Jirón	795 Stefano Vanni	643 Julien Panetier	53
Takeshi Sato	651 Lucien Dupuy	631 Antti Karttunen	607 Maurício Coutinho Neto	732 Konrad Patkowski	122