



WATOC 2017

11th Triennial Congress of the World Association
of Theoretical and Computational Chemists

27 August – 1 September 2017
Munich, Germany



POCKET PROGRAM



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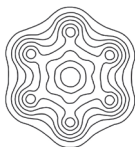
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Program – Sunday, 27 August 2017

Time	Foyer
12:00 – 15:00	Registration

Time	Philharmonic Hall
15:00 – 15:50	Opening Ceremony
15:50 – 17:10	Plenary Session A Todd Martinez Benedetta Mennucci
17:10 – 17:40	Coffee Break
17:40 – 19:00	Plenary Session B Trygve Helgaker Helmut Schwarz

Time	Foyer
19:00 – 22:00	Welcome Reception – <i>supported by BASF</i>

Program – Monday, 28 August 2017

Time	Philharmonic Hall	Carl-Orff Hall	Black Box
09:00 09:40	Plenary Session C Edward Valeev		
09:40 10:10	Coffee Break		
10:10 12:15	Invited Session 1 Peter Gill Garnet Chan Jürgen Gauss Poul Jørgensen Martin Head-Gordon	Invited Session 2 Peter Schwerdtfeger Kwang Soo Kim Jean-Luc Bredas Marco Bernardi Jochen Blumberger	Invited Session 3 Lucas Visscher Neepa Maitra Sharon Hammes-Schiffer Eberhard Gross Katarzyna Pernal
12:15 13:45	Lunch Break		
13:45 15:50	Invited Session 7 Jeremy Harvey Peter Richard Schreiner Leo Radom Yitzhak Apeloig Kendall Houk	Invited Session 8 Gustavo Scuseria Hans-Joachim Werner Örs Legeza Jeppe Olsen John Stanton	Invited Session 9 Weitao Yang Peter Pulay Henry F. Schaefer Dage Sundholm Petr Carsky
15:50 16:20	Coffee Break		
16:20 18:20	Contributed Session 1 Georg Schreckenbach Lorenzo Maschio Marek Sierka Joao B. L. Martins Wolfgang Hieringer Ralf Tonner Antti Karttunen Jon M. Matxain	Contributed Session 2 Thomas Kühne Tristan Bereau Ragnar Bjornsson Alister Page Olaf Wiest Dmitry Nerukh Laurence Leherte Xabier Lopez	Contributed Session 3 Shirin Faraji Oliver Kühn Debashree Ghosh Daniel Roca-Sanjuán Bo Durbeej László Turi Luca De Vico Valérie Brenner
18:20 20:00	Dinner Break		
20:00 22:00	Foyer		
	Poster Session 1 – supported by ACS Energy Letters		

Program – Monday, 28 August 2017

Small Concert Hall	Carl-Amery Hall	Multipurpose Room	Time
			09:00 09:40
Coffee Break			09:40 10:10
Invited Session 4 Kenneth Ruud Pekka Pyykkö Wenjian Liu Trond Saue Marcel Swart	Invited Session 5 Hiromi Nakai Nuria Lopez Tore Brinck Stuart Macgregor Michelle Coote	Invited Session 6 Odile Eisenstein Michael Buehl Gustavo Aucar Ibon Alkorta Sotiris Xantheas	10:10 12:15
Lunch Break			12:15 13:45
Invited Session 10 Kurt Kremer Florian Müller-Plathe Christoph Dellago Christine Peter Alexander Nemukhin	Invited Session 11 David Clary Irene Burghardt Roland Mitric Ivano Tavernelli Graham Worth	Invited Session 12 Benjamin Fingerhut Christel Marian Ilaria Ciofini Satoshi Maeda Henrik Koch	13:45 15:50
Coffee Break			15:50 16:20
Contributed Session 4 Manabu Sugimoto Tetsuya Taketsugu Mark Waller Seiji Mori Woo Youn Kim Anoop Ayyappan Wolfgang Quapp Michael Springborg	Contributed Session 5 Andreas Hauser Raul Alvarez-Idaboy Albeiro Restrepo Alessandro Contini Przemyslaw Dopieralski Joonkyung Jang Petra Imhof Wieslaw Nowak	Contributed Session 6 Mercedes Alonso Daniel Aravena Alexandre Magalhães Michal Straka Matthias Lein Juan F. Espinal Oscar Lung Wa Chung Amalia I. Poblador Bahamonde	16:20 18:20
Dinner Break			18:20 20:00
Foyer			20:00
Poster Session 1 – supported by ACS Energy Letters			22:00

Program – Tuesday, 29 August 2017

Time	Philharmonic Hall	Carl-Orff Hall	Black Box
09:00 09:40	Plenary Session D Giulia Galli		
09:40 10:10	Coffee Break		
10:10 12:15	Invited Session 13 Walter Thiel Stefan Grimme Frank Jensen Siewert-Jan Marrink Jan H. Jensen	Invited Session 14 Ali Alavi Seiichiro Ten-no Roi Baer David Tannor Mark Gordon	Invited Session 15 Leticia González Roland Lindh Chantal Daniel George Schatz Joseph Subotnik
12:15 13:45	Lunch Break		
13:45 15:50	Invited Session 19 Teresa Head-Gordon Jiali Gao Modesto Orozco Shina Caroline Lynn Kamerlin Helmut Grubmüller	Invited Session 20 Don Truhlar Carlo Adamo Kieron Burke G. Narahari Sastry David Sherrill	Industry Session 1 Peter Deglmann Christoph Taeschler Michael Edmund Beck Marcel Verdonk Thomas Fox
15:50 16:20	Coffee Break		
16:20 18:20	Contributed Session 7 Mario Piris Heather Kulik Pierre-Francois Loos Henk Eshuis Jiri Klimes Eduard Matito Jan Řezáč Ekaterina Pas	Contributed Session 8 Andrey Rogachev Carsten Baldauf Brian Yates Hélène Bolvin Masato Kobayashi Lubomír Rulíšek Zahra Jamshidi Jean Christophe Tremblay	Industry Session 2 Glenn Jones Hanne Falsig Martin Letz Matthias Bremer Thomas Eckl
18:20 20:00	Dinner Break		
20:00 22:00	Foyer		
	Poster Session 2 – supported by <i>The Journal of Physical Chemistry</i>		

Program – Tuesday, 29 August 2017

Small Concert Hall	Carl-Amery Hall	Multipurpose Room	Time
			09:00 09:40
Coffee Break			09:40 10:10
Invited Session 16 Joel Bowman Robert Berger R. Benny Gerber Lorenz S. Cederbaum Sergey Yurchenko	Invited Session 17 Fernando Martin Shaul Mukamel H. Bernhard Schlegel Peter Saalfank Peter Knowles	Invited Session 18 Zexing Cao Tim Clark Markus Meuwly Sereina Riniker Xuhui Huang	10:10 12:15
Lunch Break			12:15 13:45
Invited Session 21 Michele Parrinello Ulf Ryde Zhipan Liu GuanHua Chen Michele Pavanello	Invited Session 22 Elfi Kraka Gabriel Merino Raghavan B. Sunoj Gopalan Rajaraman Laura Gagliardi	Invited Session 23 Takeshi Yanai Claudia Draxl Beate Paulus Krzysztof Szalewicz WanZhen Liang	13:45 15:50
Coffee Break			15:50 16:20
Contributed Session 9 Masayoshi Nakano Carmen Herrmann Takatoshi Fujita Paula Homem-de-Mello Tangui Le Bahers Basile F. E. Curchod William Glover Matthias Stein	Contributed Session 10 Mercè Deumal Nathalie Guihery Annika Bande Martin Rahm Ian Mackinnon Fernando Ruipérez Toyokazu Ishida Eliseo Ruiz	Contributed Session 11 Ferran Feixas Snezana Zaric Vladimir Palyulin José Pedro Cerón-Carrasco Niels Hansen Janos Daru Allan East Ole Swang	16:20 18:20
Dinner Break			18:20 20:00
Foyer			20:00
Poster Session 2 – supported by <i>The Journal of Physical Chemistry</i>			22:00

Program – Wednesday, 30 August 2017

Time	Philharmonic Hall	Carl-Orff Hall	Black Box
09:00 09:40	Plenary Session E Pavel Hobza		
09:40 10:10	Coffee Break		
10:10 12:15	Invited Session 24 Alan Aspuru-Guzik Michele Ceriotti Markus Reiher Matthias Scheffler Gregory Voth	Invited Session 25 Sason Shaik Clemence Corminboeuf Julia Rice Matthias Bickelhaupt William Hase	Invited Session 26 Karsten Reuter Fabrizia Negri Mariachiara Pastore Biswarup Pathak Zhigang Shuai
12:15 13:00	Lunch Break		
13:00 20:00	Excursions		

20:00 22:00	Löwenbräukeller (Address: Nymphenburger Str. 2)
	Congress Dinner

Program – Wednesday, 30 August 2017

Small Concert Hall	Carl-Amery Hall	Multipurpose Room	Time
			09:00 09:40
Coffee Break			09:40 10:10
Invited Session 27 David Tozer Hannes Jonsson Julien Toulouse Erin R. Johnson Matthias Ernzerhof	Invited Session 28 Marcus Elstner Elena Laura Coitino Izaguirre Matthias Heyden Ville Kaila Holger Gohlke	Invited Session 29 Bogumil Jeziorski Manuel Yanez Johannes Kästner Eluvathingal D. Jemmis Péter G. Szalay	10:10 12:15
Lunch Break			12:15 13:00
Excursions			13:00 20:00
Löwenbräukeller (Address: Nymphenburger Str. 2)			20:00
Congress Dinner			22:00

Program – Thursday, 31 August 2017

Time	Philharmonic Hall	Carl-Orff Hall	Black Box
09:00 09:40	Plenary Session F Hiroshi Nakatsuji		
09:40 10:10	Coffee Break		
10:10 12:15	Invited Session 30 Filipp Furche Axel Becke Eunji Sim Andreas Görling Paul Ayers	Invited Session 31 Josef Michl Gernot Frenking Marco Nascimento Julia Contreras-García Russell J. Boyd	Invited Session 32 Chiara Cappelli Jacob Kongsted Lyudmila Slipchenko Fred Manby Kurt V. Mikkelsen
12:15 13:45	Lunch Break		
13:45 15:50	Invited Session 36 Richard Henchman Johan Aqvist Qiang Cui Pavel Jungwirth Gerhard Hummer	Invited Session 37 Marcel Nooijen Georg Kresse Silke Biermann Volker Blum Gregory Beran	Invited Session 38 So Hirata Dominika Zgid Denis Jacquemin Lucia Reining Wim Klopper
15:50 16:20	Coffee Break		
16:20 18:20	Contributed Session 12 Jan M.L. Martin Ricardo Mata Peter Nagy Graham Fletcher Jean-Philip Piquemal Joonsuk Huh Luca Frediani Sebastian Höfener	Contributed Session 13 Nick Mayhall Remco Havenith Andrzej L Sobolewski Thomas Koerzdoerfer Emanuele Coccia Robert Góra Isabelle Navizet Stefan Knippenberg	Contributed Session 14 Stella Stopkowicz Sandra Lubner Malgorzata Biczysko Takeshi Iwasa Franco Egidi Sergei Ivanov Stepan Sklenak Alfonso Hernandez-Laguna
18:20 20:00	Dinner Break		
20:00 22:00	Foyer		
	Poster Session 3 – supported by ACS Publications		

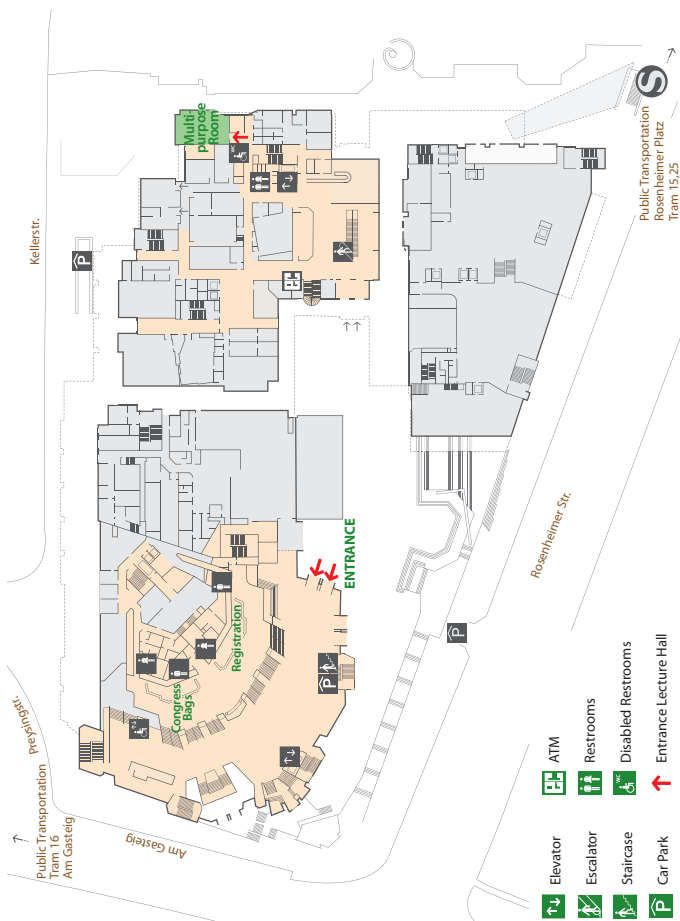
Program – Thursday, 31 August 2017

Small Concert Hall	Carl-Amery Hall	Multipurpose Room	Time
			09:00 09:40
Coffee Break			09:40 10:10
Invited Session 33 Anna Krylov Xiaosong Li Andreas Dreuw Spiridoula Matsika John Herbert	Invited Session 34 Rodney J. Bartlett Andreas Köhn Shuhua Li Jiri Pittner Ove Christiansen	Invited Session 35 Pedro Fernandes Yiqin Gao Young Min Rhee Carmay Lim David Smith	10:10 12:15
Lunch Break			12:15 13:45
Invited Session 39 Toru Shiozaki David Tew Yuki Kurashige Hans Jørgen Aagaard Jensen Piotr Piecuch	Invited Session 40 Patrick Norman Daniel Crawford Benoît Champagne Sonia Coriani Antonio Rizzo	Invited Session 41 Igor Alabugin Miroslav Urban Attila Csaszar Annia Galano Munir Skaf	13:45 15:50
Coffee Break			15:50 16:20
Contributed Session 15 Martin Kaupp Lars Goerigk Sergei Vyboishchikov Arindam Chakraborty István Mayer Fan Wang Mikael P. Johansson Ran Friedman	Contributed Session 16 Mark Iron Silvia Simon Ulrike Salzner Hong-Xing Zhang Martial Boggio-Pasqua Aurélie Perrier David Henry Thibaud Étienne	Contributed Session 17 José Enrique Barquera-Lozada Fabio Pichierri András Stirling Leonardo Belpassi Apostolos Kalemos David Wilson Ignacy Cukrowski Hugo Gattuso	16:20 18:20
Dinner Break			18:20 20:00
Foyer			20:00
Poster Session 3 – supported by ACS Publications			22:00

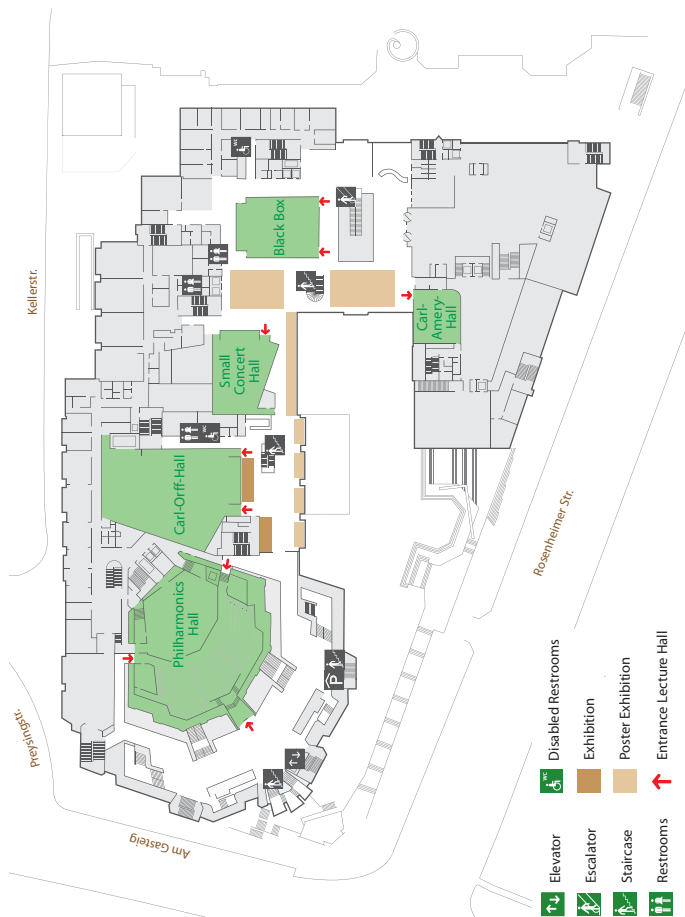
Program – Friday, 1 September 2017

Time	Philharmonic Hall
09:00 – 10:20	Plenary Session G Francesco Evangelista Johannes Neugebauer
10:20 – 10:50	Coffee Break
10:50 – 12:10	Plenary Session H Ursula Roethlisberger Frank Neese
12:10 – 12:50	Closing Ceremony and Poster Awards

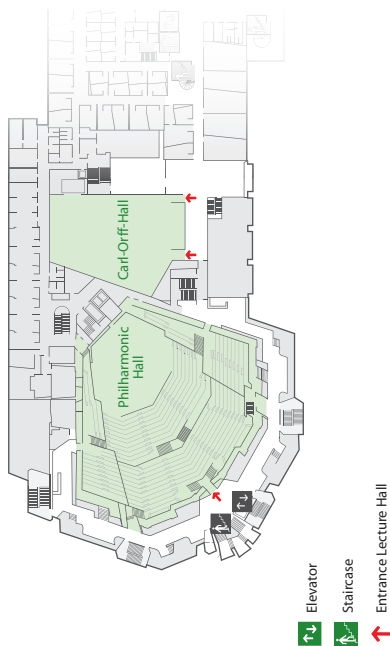
Overview – Ground Floor



Overview – First Floor



Overview – Second Floor



Restaurant Suggestions

We recommend that you call the restaurants to make a reservation. Also, at the Gasteig conference center, there will be food stations where you can purchase a small lunch or snack.

gast

Rosenheimer Str. 5, 81667 Munich

Open daily: 11:00 - 01:00

Phone: +49 (0)89 48 09 82 720

Distance: 1 min by foot

Italian and Asian cuisine

Rosi Kaffeehaus & Bar

Rosenheimer Str. 2, 81669 Munich

Open daily: 08:00 - 01:00

Phone: +49 (0)89 44 99 97 39

Distance: 2 min by foot

Modern café

Kuchlverzeichnis

Rosenheimer Str. 10, 81669 Munich

Open daily: 17:30 - 01:00

Phone: +49 (0)89 48 17 49

Distance: 3 min by foot

Traditional Bavarian food

Kam Yi

Rosenheimer Str. 32, 81669 Munich

Open daily: 11:30 - 23:30

Phone: + 49 (0)89 44 81 366

Distance: 4 min by foot

Chinese restaurant

Chez Fritz

Preysingstr. 20, 81667 Munich

Open daily (except Mondays): 17:30 - 01:00

Phone: +49 (0)89 44 87 676

Distance: 5 min by foot

French brasserie

Lollo Rosso Bar(varian) Grill

Milchstr. 1, 81667 Munich

Open daily: 17:00 - 01:00

Phone: +49 (0)89 88 56 81 31

Distance: 5 min by foot

Bavarian restaurant

L'Osteria

Innere Wiener Str. 2, 81667 Munich

Open daily: 11:00 - 00:00

Phone: +49 (0)89 62 23 28 05

Distance: 7 min by foot

Modern Italian restaurant

Hofbräukeller

Innere Wiener Str. 19, 81667 Munich

Open daily: 10:00 - 22:00

Phone: +49 (0)89 45 99 250

Distance: 7 min by foot

Bavarian restaurant with a nice beergarden

Wirtshaus in der Au

Lilienstr. 51, 81669 Munich

Open daily: 17:00 - 00:00

Phone: +49 (0)89 44 81 400

Distance: 7 min by foot

Fine Bavarian cuisine

Restaurant Del Cavaliere

Weißburger Str. 3, 81667 Munich

Open daily: 11:30 - 00:30

Phone: +49 (0)89 48 83 88

Distance: 9 min by foot

Traditional Italian restaurant

General Information

Scientific Chair

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Ludwig-Maximilians-Universität (LMU) München
Butenandtstr. 7
81377 Munich, Germany

Hosting Society

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Status: August 2017. All information is subject to change.



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