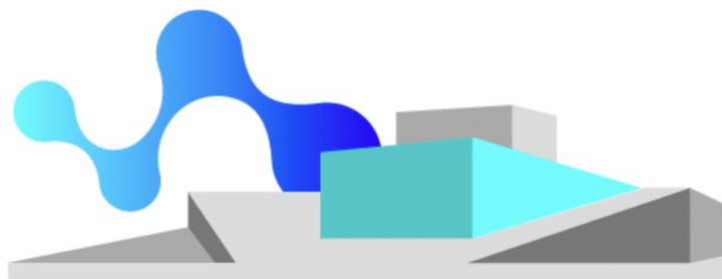


Report on the WATOC 2025 Congress Oslo June 21–27 2025

Trygve Helgaker

Hylleraas Centre for Quantum Molecular Sciences
Department of Chemistry
University of Oslo

19th December 2025



UNIVERSITETET
I OSLO



In June 2025, the 13th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC) was held at the Oslo Congress Centre, hosted by the Hylleraas Centre at the University of Oslo. The congress brought together 1,098 researchers in theoretical and computational chemistry and featured 330 oral presentations and 627 posters. Talks were given on all seven days of the week, beginning on Saturday June 21 and ending on Friday June 27. WATOC 2025 was therefore probably the longest congress ever held in the history of theoretical chemistry.

The congress consisted of two parts: the Young WATOC pre-congress on 21 June and the main WATOC congress on 22–27 June. Young WATOC was a new initiative, tried in Oslo for the first time, while the main WATOC event followed in the footsteps of previous congresses.

The WATOC Congresses, which are the largest international gatherings in theoretical chemistry are held every three years at venues selected by the WATOC Board through a competitive bidding process.

Oslo was chosen as host city only after an effort spanning several years. The first two bids, submitted at WATOC 2011 in Santiago de Compostela and at WATOC 2014 in Santiago de Chile, were unsuccessful. A third proposal, presented at WATOC 2017 in Munich, won the ballot in December 2019 to host the 2023 congress in Oslo. However, following the postponement of the Vancouver congress from 2020 to 2022 because of the COVID-19 pandemic, the congress in Oslo was rescheduled from 2023 to 2025.

Organization

The Oslo congress was chaired by Trygve Helgaker, former director and now adjunct member of the Hylleraas Centre, who also served on the Local Congress Committee. This committee comprised all Hylleraas PIs in Oslo—David Balcells, Michele Cascella, Abril Castro, Simen Kvaal, Ainara Nova, Thomas Bondo Pedersen, Simen Reine, and Erik Tellgren plus researcher Sigbjørn Løland Bore and affiliates Odile Eisenstein and Einar Uggerud. Simen Reine and Erik Tellgren served as congress secretaries. The Young WATOC conference was chaired by Abril Castro and Ainara Nova.

To support the planning and execution of WATOC 2025, the organizers partnered with the Professional Congress Organizer (PCO) Gyro Conference. Financial security was provided by the Faculty of Mathematics and Natural Sciences, which guaranteed coverage of any potential loss in exchange for receiving any surplus—an arrangement essential for moving forward with a congress of this scale. The contract concluded with Gyro was first approved by the Faculty.

Venue

The Oslo Congress Centre was selected as the venue for WATOC 2025 due to its central location and its capacity to host roughly 1,100 participants across five parallel sessions. When the first bid was prepared in early 2011, no WATOC congress had yet exceeded 1,000 participants. Although this later changed with WATOC 2011 (1,353 participants) and WATOC 2017 (1,520), no efforts were made to secure a larger venue as it was assumed that attendance would be lower than at these more centrally situated congresses. In addition, venues with greater capacity would have required moving the event outside Oslo city centre.



Oslo Congress Hall with WATOC banner. Photo: Trygve Helgaker

Hylleraas Crew

To ensure the smooth daily operation of the congress, the WATOC Crew, consisting of 33 young members of the Hylleraas Centre, played an important role. Dressed in bright orange T-shirts, the Crew members were easy to spot by participants and ready to assist with any matter. They helped with registration and were present at each lecture, helping to keep sessions on schedule and managing microphone distribution during discussions.

In addition to their logistical duties, the Crew organized the social program, which included morning runs, walks, and sauna sessions, as well as Wednesday-afternoon activities such as hikes, guided walking tours, and an evening networking event at Røør Bar.

The Crew consisted of the following members of the Hylleraas Centre: Derya Aricigil, Michael Augello, Lucas Bitencourt Theodoroviez, Marco Bortoli, Klara Elvira Haug Boström, Ning Cao, Henrique Musseli Cezar, Aurore Evelyne Francine Denjean, Mohamed Eid Ahmed Safy, Sondre Eliasson, Hanne Jeeyung Eriksen, Håkon R. Fredheim, Miguel Angel Gaona Fernandez, Gabriel Gerez, Hanan Gharayba, Lucia Moran Gonzalez, Jose Alberto Guerrero Cruz, Helena Hradiska, Catherine Hughes, Hannes Kneiding, Håkon Emil Kristiansen, Morten Ledum, Manuela Leal Nader, Oliver Macphail Bohle, Daniel Marke, Joel Ormala, Quentin Pitteloud, Mauricio Portolli Franco, Tonje Reinholdt Haugen, Jordan Rio, Inga Schmidtke, Simon Elias Schrader, and Øystein Senstad.

The crew was divided into three equally large teams, each led by one of the three team leaders: Morten Ledum, Lucia Moran Gonzalez, and Henrique Musseli Cezar. Marco Bortoli acted as the official WATOC photographer.



Registration and participants

A detailed budget for the congress was prepared in collaboration with our PCO, with the objective of keeping registration fees comparable to those of previous WATOC meetings. The regular registration fee was set at NOK 8,600 (full) and NOK 7,800 (early-bird), while the student fee (for master's and PhD students) was NOK 4,800 (full) and NOK 4,200 (early-bird). These fees included participation at Young WATOC, for all interested. The Registration fee was waived for members of the WATOC Scientific Board (in accordance with WATOC statutes) and for a handful of other participants.

Registration opened in October 2024. Interest in WATOC 2025 exceeded expectations: the congress reached full capacity at the close of early-bird registration on 28 February, with 1,150 participants registered. Only 75 participants (all invited speakers) paid the full fee.

Due to various circumstances—including the temporary closure of airspace in parts of the Middle East in June—approximately 50 registered participants cancelled their attendance, resulting in a final total of 1,098 registered participants. The registration fees of those unable to attend were refunded, subject to a cancellation charge, in November 2025.

WATOC 2025 attracted theoretical chemists from all parts of the world: 772 from Europe, 143 from Asia, 127 from North America, 30 from Latin America, 13 from Oceania, 8 from the Middle East, and 4 from Africa. The ten countries with the largest number of participants were Germany (161), the United States (103), Norway (78), Spain (65), the United Kingdom (63), Italy (54), France (47), China (45), Switzerland (45), and Japan (40).

Students accounted for one third of all participants (384 in total).



Crew members Michael Augello (left) and Sondre Eliasson (right) assisting at registration. Photo: Marco Bortoli



Crew member Manuela Leal Nader with countdown cards. Photo: Marco Bortoli

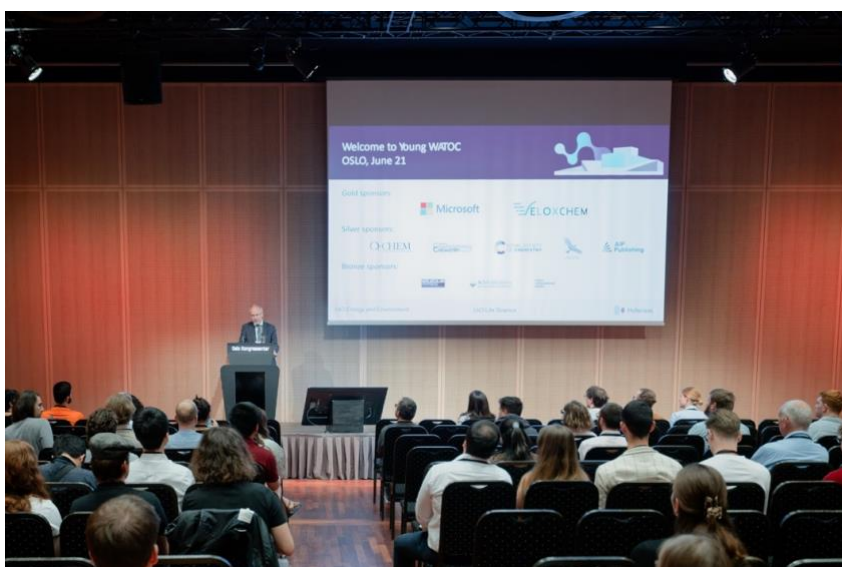
Young WATOC

Young WATOC was held on Saturday, June 21, one day before the start of the main conference. All speakers were either registered PhD students or researchers who had defended their theses in 2020 or later.

Selecting speakers for Young WATOC proved to be a challenging task: 102 highly competitive abstracts were submitted for 18 available slots. The speakers were selected based on the quality of the research, while maintaining a balanced representation across research subfields, geographical regions, and gender.

The Young WATOC pre-conference, which was open to all participants of WATOC, was attended by about 300 participants. In the evening on June 21, 230 attendees joined the BBQ at Skullerudstua on the outskirts of Oslo, near Østmarka.

The Young WATOC pre-congress was well received and was highlighted by the WATOC President at the closure as a highly successful new component of the congress, to be continued at the next WATOC Congress in Mérida, Mexico, in January 2028.



Trygve Helgaker opening Young WATOC. Photo: Marco Bortoli



Young WATOC Chairs Ainara Nova (left) and Abril Castro (right). Photo: Marco Bortoli



Question time at Young WATOC. Photo: Marco Bortoli



Young WATOC BBQ at Skullerudstua on Saturday. Photo: Marco Bortoli

Program of the main WATOC congress

The main WATOC event began with official opening at 3 pm on Sunday June 21 and ended with official closing at 11:40 on Friday June 27. The scientific program consisted of six plenary sessions, each featuring two speakers (12 plenary speakers in total), and 75 parallel sessions, each with four speakers (300 speakers in total).

For logistical reasons, the plenary and parallel sessions were scheduled on separate days (see chart). The parallel program consisted of five concurrent streams, each comprising five sessions with four talks per session—making a total of 100 talks per day. On the same days, evening poster sessions were held, each featuring more than 200 presenters.

Excursions were scheduled for Wednesday, after four morning plenary lectures.

	Sun		Mon	Tue	Wed	Thu	Fri
15:00	Opening	08:30	Parallel	Parallel	Plenary	Parallel	Plenary
15:40	Plenary	09:50	Break	Break	Break	Break	Break
17:00	Break	10:20	Parallel	Parallel	Plenary	Parallel	Plenary
17:30	Plenary	11:40	Lunch	Lunch	Excursions	Lunch	Closing
18:50	Mingling	13:20	Parallel	Parallel		Parallel	
		14:40	Break	Break		Break	
		15:10	Parallel	Parallel		Parallel	
		16:30	Break	Break		Break	
		17:00	Parallel	Parallel		Parallel	
		18:20					
		20:00	Poster	Poster	Banquet	Poster	

Opening of main congress

After a welcome address by congress chair Trygve Helgaker, the audience enjoyed an engaging musical interlude by the trio Øyonn Groven Myhren, Knut Skrindo, and Ulf-Arne Johannessen, who presented Norwegian folk music and dance. The performance culminated in a *hallingkast*—a traditional dance feat in which the performer kicks down a hat held on a stick more than two meters above the floor—to great applause from the audience.

Following their performance, the congress was officially opened by the Rector of the University of Oslo, Professor Svein Stølen, himself a chemist and a former colleague of the congress chair. After an address by WATOC President Peter Gill, the musical trio returned for a second performance, after which the chair presented some practical information for participants.

The opening session was led by Einar Uggerud.

After the four plenary lectures given after the opening, attendees gathered for the opening reception in the main foyer of the congress centre.



Audience at WATOC opening ceremony. Photo: Trygve Helgaker



Musical interlude. Øyonn Groven Myhren (left) and Knut Skrindo (right). Photos: Marco Bortoli



Rector Svein Stølen opening WATOC 2025. Photo: Marco Bortoli



Opening reception. Photo: Marco Bortoli



Opening reception. Photo: Marco Bortoli

Plenary sessions

Of the twelve plenary slots, eight were reserved for the Schrödinger and Dirac medallists for 2021–2024. As Schrödinger medallist Yitzhak Apeloig was unable to attend, a total of five plenary speakers were selected by the local organizing committee, aiming for a balanced representation of scientific fields, gender, and geography while maintaining the highest scientific standards. The plenary lectures, which were held in the main congress hall, were well attended and well received.

The first four plenary lectures were presented between the opening and the reception. The first speaker was Michele Parrinello, in whose honour a special thematic session titled *Forty Years of Ab Initio Molecular Dynamics* was later held, celebrating the pioneering contributions of Roberto Car and Michele Parrinello to molecular dynamics.



Plenary speaker Michele Parrinello, Istituto Italiano di Tecnologia, Genoa, with chair Odile Eisenstein. Photo: Marco Bortoli



Miroslav Urban, Comenius University, questioning Michele Parrinello. Photo: Marco Bortoli

Parallel sessions

Each parallel session consisted of four thematically related presentations. With the exception of the final session on each day, each session lasted 80 minutes and included two 25-minute invited lectures followed by two 15-minute invited communications. The last parallel session of each day lasted 90 minutes, comprising three invited lectures and one invited communication. In total, the parallel sessions featured 165 lectures and 135 communications.



Audience in Hall B. Photo: Marco Bortoli

Selection of speakers

The speakers for the longer lectures were invited directly by the organizers, while those for the shorter communications were selected based on submitted abstracts. According to the WATOC statutes, members of the WATOC Board are entitled to speak at the congress. In total, 25 presentations (15 lectures and 10 communications) were given by Board members.

Designing a high-quality and well-balanced scientific program proved both time-consuming and challenging. The task was undertaken by the local organizing committee, with valuable input from an international Scientific Advisory Committee (SAC) comprising 32 prominent scientists from 18 countries, representing all major areas of theoretical chemistry.

The process began with defining the scientific themes or subfields to be represented at the congress. For each such theme, a provisional number of sessions was allocated to guide the invitation process. By the end of July 2024, an initial list of 320 potential speakers had been compiled, with information on their research areas, affiliations, publications (number of publications, citations, H-index), with links to home page and Google Scholar or ResearchGate. Of these, 240 were proposed by members of the SAC

and 80 by the local organizers. Over the next half year, the list was expanded to nearly 450 potential speakers as additional suggestions were received from the organizing committee and other sources.

Invitations for the 25-minute lectures began in September 2024 and were issued gradually through the autumn to ensure balanced representation across subfields, countries, and gender. By the end of the year, 139 speakers had accepted and 13 had declined the invitations. No further invitations for 25-minute lectures were issued at this stage, to allow for more flexibility when composing the thematic sessions later.

Speakers for the 15-minute communications were selected from the 416 abstracts submitted for scrutiny by March 15. In addition to considerations of quality, geography, and gender, an important consideration was to assemble coherent sessions, thematically aligned with the invited speakers already confirmed. To achieve coherence, several speakers for communications were promoted to lectures. The list of speakers for 165 lecturer and 135 communication speakers was complete by mid-May—only one month before the opening of the congress.

All invitations to speakers were sent personally by the congress chair, who also handled all subsequent correspondence with the speakers. With only a handful of exceptions, the speakers received no financial support from the organizers.



Marco Nacsimento, Federal University of Rio de Janeiro, lecturing in Hall B. Photo: Marco Bortoli

Construction of thematic program

Constructing the 75 thematic sessions was challenging, not least because overlaps between related sessions had to be avoided and since many speakers had limited availability, creating altogether over 60 individual scheduling restrictions. The schedule was completed by late May. The number of sessions for each theme was as follows: electronic structure 17, biosystems 11, catalysis & reactivity 11, energy & materials 7, spectroscopy 7, machine learning 6, chemical structure & bonding 5, quantum dynamics 5, computing & software 3, exotic systems 1, molecular dynamics 1, teaching & education 1.

To ensure a smooth running of the congress, a final confirmation was requested from each speaker—a laborious, iterative process due to changing travel plans and slow responses. As a result, the congress ran smoothly as planned, with only one adjustment because of a last-minute change in travel plans.

The 75 chairs needed for the parallel sessions were invited once the session schedule was finalized, selected among the participants.

Monday 23 June

Session A1 – 8:30	Session B1	Session C1	Session D1	Session E1
CATALYSIS & REACTIVITY Reactants, reactions, and catalysis Kevin Naidoo	ELECTRONIC-STRUCTURE THEORY Green's function methods Andreas Görling	BIOSYSTEMS Cheminformatics & medicinal chemistry Stacey Wetmore	COMPUTING & SOFTWARE Quantum computing Ivan Kassal	CHEMICAL STRUCTURE & BONDING Conjugated systems Peter Schreiner
Raghavan Sunoj	963 Dominika Zgid	924 Jean-Louis Reymond	986 Birgitta Whaley	919 Debashree Ghosh
Stuart Macgregor	926 Wim Klopper	458 Jan Rezáč	480 Artur Izmaylov	131 Abhik Ghosh
Ashique Lal	207 Marios-Petros Kitsaras	124 Elfi Kraka	130 Davide Castraldo	327 Martin Rahm
Boris Maryasin	127 Arno Förster	572 Jean-Philip Piquemal	699 Karl Michael Ziemis	260 Takafumi Shiragawa
313				
Session A2 – 10:20	Session B2	Session C2	Session D2	Session E2
MACHINE LEARNING ML for simulations Heather Külik	CATALYSIS & REACTIVITY Surfaces and heterogeneous catalysis Angel Martin Pendás	ELECTRONIC-STRUCTURE THEORY Numerical methods and techniques Stefan Grimme	BIOSYSTEMS Macromolecules Benedetta Mennucci	ELECTRONIC-STRUCTURE THEORY Ultrahigh accuracy and QED Fritz Schaefer
Gábor Csányi	967 Philippe Sautet	873 Peter Gill	953 Lynn Kamerlin	45 Trond Sæue
Alexandro Tsuchenko	995 Níria López	972 Luisa Fredini	696 Subha Kalyanamoorthy	653 Jacob Komasa
Jelle Vekeman	785 Christopher Stein	287 Eduard Matito	157 Xiang Sheng	196 Ádám Margócsy
Michael Gillhofer	317 Mireia Segadó-Centellas	716 David Sherrill	136 Adil Kabylda	547 Pekka Pyykkö
486				
Session A3 – 13:20	Session B3	Session C3	Session D3	Session E3
ELECTRONIC-STRUCTURE THEORY Coupled-cluster theory Jürgen Gauss	ENERGY & MATERIALS Condensed systems Yi Qin Gao	CATALYSIS & REACTIVITY Nonadiabatic reaction design Vidar Remi Jensen	QUANTUM DYNAMICS Nonadiabatic dynamics Ove Christiansen	BIOSYSTEMS Macromolecules Elfi Kraka
Piotr Piecuch	923 Francesco Paesani	752 Yousung Jung	441 Alicia Palacios	804 Ferran Feixas
Henrik Koch	862 Damien Laage	918 Jan H. Jensen	440 Jian Liu	86 Tage Demissie
Karol Kowalski	199 Jochen Blumberger	54 Kevin Naidoo	171 Peter Schürger	166 Petra Imhof
Francesco Evangelista	348 Marco Nascimben	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 Explicit correlation Wim Klopper	MACHINE LEARNING ML for chemical reactions Sigbjørn Laland Børre	BIOSYSTEMS Macromolecules Qiang Cui	CHEMICAL STRUCTURE & BONDING Early elements Gabriel Merino	QUANTUM DYNAMICS Ultrafast dynamics Thomas Bando Pedersen
Seichiro Ten-no	874 Boris Kozinsky	971 Modesto Orozco	819 Miroslav Urban	270 Françoise Remacle
Ali Alavi	853 Fernanda Duarte	842 Alessandra Magistrato	202 Ed Jemmis	163 Michal Repisky
Eva Zausasana Mihálka	470 Joakim Jasthi	246 Mariastella Cascone	544 Celina Sikorska	738 H. Bernhard Schlegel
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 Density-functional development Weitao Yang	MACHINE LEARNING ML for chemical design Clémentine Corminboeuf	COMPUTING & SOFTWARE Quantum computing David Paskalis	QUANTUM DYNAMICS Ultrafast dynamics Federica Agostini	CATALYSIS & REACTIVITY Electrochemistry and related Cristina Trujillo
Martin Head-Gordon	957 Clémentine Corminboeuf	446 Ivan Kassal	356 Fernando Martín García	663 Samira Siahrostami
Erin Johnson	505 Anatole von Lilienfeld	442 Marco Govoni	1007 Ove Christiansen	959 Maria Besora
Fritz Schaefer	687 Konstantinos Vogiatzis	10 Maria-Andreea Filip	419 Jiji Vanček	691 Tangui Le Bahers
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 Surfaces and heterogeneous catalysis Stuart Macgregor	ELECTRONIC-STRUCTURE THEORY Many-body methods & NCI Seichiro Ten-no	BIOSYSTEMS Bio/nanoscience Michele Casella	ELECTRONIC-STRUCTURE THEORY Relativistic quantum chemistry Trond Sæue	SPECTROSCOPY Polarization models Russell Boyd
Anastassia Alexandrova	38 Katarzyna Pernal	875 Daan Frenkel	703 Wenjian Liu	436 Benjamin Stamm
Ataulpa Braga	901 Janus Juul Eriksen	810 Wataru Shinoda	782 Jürgen Gauss	438 Kaline Coutinho
Mikhail Polyanski	353 Karline Boese	443 Achutha Kumar Dutta	97 Achutha Kumar Dutta	215 Cedric Dongmo Fomthum
Basil Raju	47 Andreas Hansen	121 João Coimbra	587 Erik Donovan Hedegård	497 Tommaso Nottoli
305				
Session A2 – 10:20	Session B2	Session C2	Session D2	Session E2
CATALYSIS & REACTIVITY Molecular and reaction design Odlie Eisenstein	ENERGY & MATERIALS Materials and energy Erica González	ELECTRONIC-STRUCTURE THEORY Berry phase & complex wave functions Henrik Koch	QUANTUM DYNAMICS Ultrafast dynamics Fernando Martín García	BIOSYSTEMS Bio/nanoscience Modesto Orozco
Satoshi Maeda	307 Laura Gagliardi	702 Hardy Gross	648 Federica Agostini	388 Biswarup Pathak
Markus Reiher	80 Elena Besley	763 Joseph Schmitz	666 Morgane Vacher	820 Matteo Dal Peraro
Derek Ahneman	161 Tim Kowalczyk	239 Ansgar Pausch	581 Yi Zhao	720 Gioacchino Schifino
Giovannimaria Piccini	698 Shubhaji Das	68 Bang Huynh	191 Angela Wilson	680 Samaneh Davoudi
79				
Session A3 – 13:20	Session B3	Session C3	Session D3	Session E3
ELECTRONIC-STRUCTURE THEORY Density-functional development Miroslav Urban	MACHINE LEARNING ML for chemical reactions Francesco Paesani	MOLUCULAR DYNAMICS Honorary session: 40 years of AIMD Matteo Dal Peraro	QUANTUM DYNAMICS DMRG and MCTDH Françoise Remacle	CHEMICAL STRUCTURE & BONDING f-block elements Pekka Pyykkö
Kieron Burke	922 Teresa Head-Gordon	847 Roberto Car	987 Irene Burghardt	666 Karin Fink
Eunji Sim	807 Dennis Salaub	91 Ursula Rothlisberger	960 Zhigang Shuai	773 Miho Hatanaka
Jacques Desmarais	128 Jeri Bulis	478 Mark Tuckerman	395 Yuki Kurashige	56 Sergey Varganov
Priya Priya	692 Haobo Li	26 Amin Alibakhshi	771 Henrik Larsson	174 Meagan Oakley
700				
Session A4 – 15:10	Session B4	Session C4	Session D4	Session E4
CATALYSIS & REACTIVITY Surfaces and heterogeneous catalysis Philippe Sautet	SPECTROSCOPY Methods for excited electronic states Philippe Sautet	BIOSYSTEMS Multiscale modelling Piotr Piecuch	ELECTRONIC-STRUCTURE THEORY Strong correlation & entanglement Marco Nascimben	ENERGY & MATERIALS Condensed systems Marco Nascimben
Annabella Selloni	748 Emmanuel Fromager	755 Benedetta Mennucci	832 Shuhua Li	881 Nicola Gaston
Akira Nakayama	681 Weitao Yang	956 Paula Homem-de-Mello	686 Mario Piris	16 Pavel Jungwirth
Seungjae Kwak	437 Momir Malis	787 Yingjie Wang	117 Jiji Pittner	77 Sheh-Yi Shue
Francisco Vñhes Solana	89 Lars Goerik	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 Cheminformatics & medicinal chemistry Ursula Rothlisberger	ELECTRONIC-STRUCTURE THEORY Methods for larger systems David Sherrill	CATALYSIS & REACTIVITY Reactants, reactions, and catalysis Annia Galano	SPECTROSCOPY Circular dichroism Kenneth Ruud	EXOTIC SYSTEMS Strong fields and high pressure Peter Schwerdtfeger
William Jorgensen	808 Christian Ochsenfeld	952 David Wales	969 Daniel Crawford	757 Stella Stopkowitz
Zoe Courina	981 Hiromi Nakai	723 Felu Meseras	673 Luuk Visser	814 Andrew Wibowo-Teale
Stacey Wetmore	321 Philipp Lippari	626 Sebastian Kusch	2 Wandchen Liang	245 Erik Zurek
Christoph Riplinger	714 Mariastella Alessio	187 Masataka Nagakawa	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 Methods for periodic systems Christian Ochsenfeld	SPECTROSCOPY Methods for excited states Emmanuel Fromager	BIOSYSTEMS Multiscale modelling Stefano Vanni	CHEMICAL STRUCTURE & BONDING Analysis Henry Rzepa	ENERGY & MATERIALS Photophysics and photochemistry Zhigang Shuai
Georg Kresse	831 Julia Westermayr	364 Qiang Cui	689 Matthias Bickelhaupt	670 Dage Sundholm
Lin Lin	571 Hannes Jørgensen	660 Garnet Chan	872 Frank de Proft	813 Jing Ma
David Tew	870 Thomas Froitzheim	81 Andrea Pérez-Villa	504 Inbal Tzvi-Arad	749 Dana Nachtigallová
Philip Hoggan	13 Elfi 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 Simpler model systems Anna Krylov	CATALYSIS & REACTIVITY Reactants, reactions, and catalysis Manuel Yañez	BIOSYSTEMS Multiscale modelling Garnet Chan	ENERGY & MATERIALS Photophysics and photochemistry Dage Sundholm	COMPUTING & SOFTWARE Software Daniel Crawford
Stefan Grimme	825 Evert Jan Meijer	943 Carme Rovira	863 Kumar Vanka	899 Patrick Norman
Peter Schwerdtfeger	92 Bastian Skjeltved	715 Marco De Vivo	817 Leticia González	964 Susi Lehtola
Per Siegbahn	212 Amalia Poblador Bahamonde	880 Stefano Serapian	120 Enrico Tapavicz	523 John Herbert
Itai Panas	679 Zhixuan Song	654 Allison Keys	226 Enrique Manuel Arpa	411 Alexander Stark
513				
Session A3 – 13:20	Session B3	Session C3	Session D3	Session E3
ELECTRONIC-STRUCTURE THEORY Density-functional development Jiali Gao	CATALYSIS & REACTIVITY Molecular and reaction design Ainsara Nova	MACHINE LEARNING ML for simulations Konstantinos Vogiatzis	SPECTROSCOPY Rotovibrational spectra Sonia Coriani	TEACHING & EDUCATION Teaching & education Trygve Helgaker
Stefan Vuković	837 Anina Galano	508 Yi Luo	737 Attila Császár	931 Anders Maithe-Sørensen
Martin Knapp	661 Vidar Rami Jensen	948 Yi Qin Gao	882 Guntram Rauhut	106 Peter Taylor
Hans Jørgen Aa. Jensen	457 Cristina Trujillo	36 Amanda Ardisiaco	537 Ayaki Sunaga	735 Erik Andree
Aaron Garrison	159 Wataru Matsuo	237 Krzysztof Szalewicz	730 Frederik Tielens	72 Henry Rzepa
12				
Session A4 – 15:10	Session B4	Session C4	Session D4	Session E4
CATALYSIS & REACTIVITY Reactants, reactions, and catalysis Felix Meseras	ENERGY & MATERIALS Materials and energy Evert Jan Meijer	ELECTRONIC-STRUCTURE THEORY Optimization in quantum chemistry Erik Telgren	MACHINE LEARNING ML for electronic structure Paola Gori-Giorgi	SPECTROSCOPY Positrons & weak interactions Edi Mitrop
Jin Wen	800 Debra Bernhardt	751 Eric Cancos	742 Paola Gori-Giorgi	867 Gustavo Aucar
Fahmi Him	928 Sara Bonelli	827 Roland Lindh	672 Matthias Kick	233 Robert Berger
Johannes Hoja	575 Virginia Carnevali	538 Giovanni Scalmani	619 Angel Martín Pendás	58 Dermot Green
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 Spectroscopy & energy surfaces Abril Castro	ELECTRONIC-STRUCTURE THEORY Beyond standard DFT Paola Gori-Giorgi	ENERGY & MATERIALS Materials and energy Laura Gagliardi	BIOSYSTEMS Bio/nanoscience Carme Rovira	CHEMICAL STRUCTURE & BONDING Coordination chemistry Ed Jemmis
Sonia Coriani	925 Paul Ayers	733 Marie-Liesse Doublet	966 Sergio Pantano	417 Gabriel Merino
Anna Krylov	382 Jiali Gao	904 Emi Minamitani	93 Cristiana Di Valentin	794 Jeanet Conrade
Ide-Marie Hayvik	721 Andreas Görling	220 Gloria I. Cárdenas-Jirón	795 Stefano Vanni	643 Julien Panetier
Takeshi Sato	651 Lucien Dupuy	651 Antti Karttunen	607 Mauricio Coutinho Neto	732 Konrad Patkowski
122				

Some speakers who were unable to attend for different reasons beyond their control were allowed to present pre-recorded talks at the congress.



Raghavan B. Sunoj, IIT Bombay, presenting a recorded talk in Hall A. Photo: Marco Bortoli

Lecture halls

For the parallel sessions, the main lecture hall was divided into three rooms with capacities of 620, 378, and 252 participants. In addition, two smaller lecture halls were used—one seating about 150 participants (plus roughly 50 standing in the aisles) and another accommodating about 100 participants, with an adjacent overflow room providing space for an additional 60 attendees via video transmission. When the final WATOC bid was made, an additional Forum Hall with a capacity of 170 was available, but it was demolished during the pandemic, making the solution with dual-room and video solution necessary.

The allocation of sessions to lecture halls was guided by the participants' stated areas of interest during registration and proved largely successful. A few sessions became overcrowded, giving the speakers the thrill of addressing a packed audience, with some attendees even standing.

Technical support

For the smooth running of the sessions, one crew team (eleven people) was responsible for all five parallel streams at any given time, providing technical support such as downloading slides before sessions, managing time, and handling microphones during presentations. To facilitate timekeeping, three large timing boards were designed and displayed by a crew member at appropriate intervals. With only a few exceptions, time management was excellent, keeping all sessions well synchronized.

Likewise, support provided by the Oslo Congress Centre in connection with lectures were top notch, resulting in very few glitches in the sessions.

10 minutes left
of total time

5 minutes left
Time for discussion

STOP!
Time is up



Erik Tellgren and Crew members in the technical preparation room. Photo: Marco Bortoli



Crew leader Henrique Cesar assisting Mauricio Coutinho-Neto of Federal University of ABC in Hall D. Photo: Marco Bortoli

Speaker statistics

The total number of speakers was 330. Of these, 18 were Young WATOC speakers, 12 were plenary speakers, 165 were speakers giving 25-minute presentations, and 135 were speakers giving 15-minute presentations. The statistics below are aggregated across all categories of speakers. In cases of dual affiliation, a value of 0.5 has been assigned to each corresponding country or region.

Number of speakers by region: Europe 190.5, North America 69, Asia 42.5, Latin America 11, Oceania 8, Middle East 6, Africa 3.

Number of speakers by country: USA 59, Germany 29.5, UK 19.5, Switzerland 18, France 16, Italy 16, China 15.5, Spain 15, Japan 13, Canada 10, Belgium 9, Sweden 9, Norway 8, Denmark 7, Netherlands 7, Australia 6, Austria 6, Israel 5, South Korea 5, Finland 4.5, Hungary 4.5, Poland 3, Brazil 3, Iceland 2, Luxembourg 2, Mexico 2, New Zealand 2, Singapore 2, South Africa 2, Argentina 1, Botswana 1, Chile 1, Greece 1, Iran 1, Portugal 1, Taiwan 1, Uruguay 1.

In total, 37 countries and about 230 institutions were represented at WATOC, from all parts of the world. No speakers were invited from the host institution (Department of Chemistry, University of Oslo). Overall, 99 (30%) of the speakers were female.



First coffee break between parallel sessions on Tuesday. Photo: Trygve Helgaker

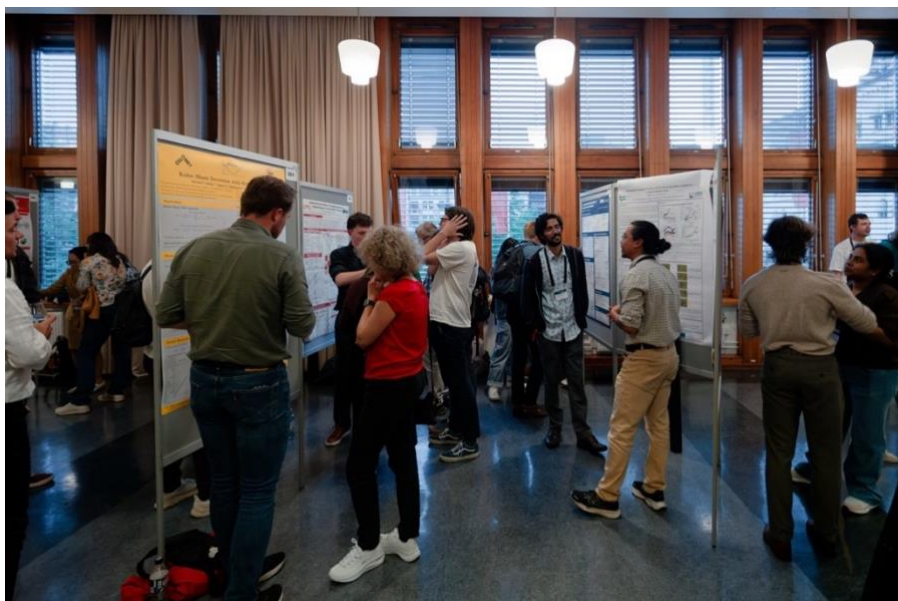
Poster sessions

A total of 627 posters were presented in order of registration across three poster sessions, each featuring more than 200 posters. The sessions were well attended and crowded but no more than is typical for large international congresses.

Ten poster prizes were awarded at the congress, judged by a panel of 21 anonymous reviewers. The prizes included three awards from the *Journal of Computational Chemistry* (each consisting of a €200 gift card), three from the Royal Society of Chemistry (social media promotion and a £150 book voucher), one from the *Journal of Chemical Theory and Computation* (one-year ACS membership and \$250), and three from the Hylleraas Centre (*reMarkable tablets*). The prizes were presented to the winners at the closing ceremony of the congress.



Monday poster session. Photo: Marco Bortoli



Tuesday poster session. Photo: Marco Bortoli

Conference banquet

The conference banquet on Wednesday, attended by 683 participants and accompanying persons, was hosted by Einar Uggerud, who welcomed the guests. The main course featured moose meat, a Norwegian specialty. After the main course, Trond Saue, now based in Toulouse but educated in the theory group in Oslo, addressed the dinner guests and introduced the musical entertainment. The performance was given by tenor Marius Roth Christensen, accompanied by a pianist Ivar Anton Waagaard. The traditional Norwegian “thanks for the dinner speech” was given by Ole Swang.

The congress dinner was open to all participants and accompanying persons, for a fee of NOK 1,150 per person. The fee was reduced by NOK 500 for WATOC Scientific Board.



Banquet dinner in plenary lecture hall. Photo: Marco Bortoli



Banquet menu. Photo: Marco Bortoli



Banquet dinner. Photo: Marco Bortoli



Banquet dinner. Photo: Marco Bortoli



Marius Roth Christensen accompanied by Ivar Anton Waagaard at the banquet. Photo: Marco Bortoli

Social activities

A varied programme of social activities was organized in connection with the congress, with the main events taking place on Wednesday afternoon. Participants could join a guided tour of the National Museum, a hiking excursion to Vettakollen, a ferry trip to the island of Hovedøya, or a guided historic walking tour in the city centre. In addition, a number of recommended activities were highlighted for individual visits, including the Norwegian Museum of Science and Technology, the Fram Museum, the Norwegian Museum of Cultural History, and the Munch Museum.

To promote informal networking and well-being, morning run, morning walk, and morning sauna sessions were organized every day from Monday to Friday at 7:00 am, all free of charge. Participants were offered a 20% discount on the Oslo Pass, a tourist card providing free access to a wide range of attractions as well as free public transportation.



Morning run led by Crew members Morten Ledum and Håkon Fredheim. Photo: Marco Bortoli

Although the weather during the congress was mixed, typical of Oslo summers, we were fortunate to have excellent weather for the excursion.

Closing Ceremony

The closing ceremony took place after two plenary sessions on Friday morning. During the ceremony, ten poster prizes were first presented by the leader of the Poster Prize Committee, David Balcells. The chair of the conference then addressed the audience, expressing gratitude to everyone involved—including the local organizing committee, the Hylleraas Crew, and the international Scientific Advisory Board and the WATOC organization. This was followed by a presentation from Gabriel Merino, introducing WATOC 2028, to be held in Mérida, Mexico, from 9 to 14 January 2028.

The congress was formally closed by WATOC President Peter Gill, who praised the conference as “outstanding” and highlighted Young WATOC as a very valuable addition that will continue at the next Congress. Finally, Peter Gill introduced the incoming WATOC President, Martin Head-Gordon, who delivered the concluding address to the audience. The closing was led by Einar Uggerud.



Audience at the conference closing ceremony. Photo: Marco Bortoli



Poster Prize winners flanked by Peter Gill (left) and Trygve Helgaker (right). Photo: Cathrine Strøm



The WATOC crew receives well-deserved thanks at the conference closing. Photo: Cathrine Strøm



Local Organizing Committee at the conference closing. Photo: Cathrine Strøm



Incoming WATOC President Martin Head-Gordon (left) and outgoing President Peter Gill (right) at the conference closing ceremony. Photo: Macro Bortoli

Sponsors

The WATOC Congress was supported by a range of sponsors. We were fortunate to have two Gold Sponsors — Microsoft and VeloxChem — along with five Silver Sponsors: AIP Publishing (*Journal of Chemical Physics*), FACCTs (ORCA), Wiley (*Journal of Computational Chemistry*), Q-Chem, and the Royal Society of Chemistry (*Chemical Science*, *Digital Discovery*, *Physical Chemistry Chemical Physics*). Three organizations joined as Bronze Sponsors: ACS Publications (*Journal of Chemical Theory and Computation*), Springer Nature (*Nature Computational Science*), and Taylor & Francis (*Molecular Physics*).



We also received support from the French non-profit organization Young Theoretician Chemists Association (YTCA) at the University of Montpellier, as well as generous local support from UiO: Energy and Environment and UiO: Life Science. The Hylleraas Centre provided additional contributions, and the Faculty of Mathematics and Natural Sciences guaranteed coverage of any potential financial losses.

Exhibitors

The exhibitors comprised four software companies (FACCTs, ioChem-BD, Q-Chem, and SCM) and two scientific publishers (AIP and RSC). Their booths were located in the main foyer of the congress hall and remained open throughout all breaks.



Software developer David Ormrod Morleh from Software for Chemistry & Materials (SCM) at the exhibition booth. Photo: Marco Bortoli

Financial Framework

Organizing a congress on the scale of WATOC 2025 within a public institution poses specific financial challenges, in particular related to VAT handling and the Norwegian regulations on public procurement. Under a traditional organizational model, these constraints would have resulted in double VAT exposure and substantially more complex contracting with multiple suppliers, ultimately increasing costs for participants.

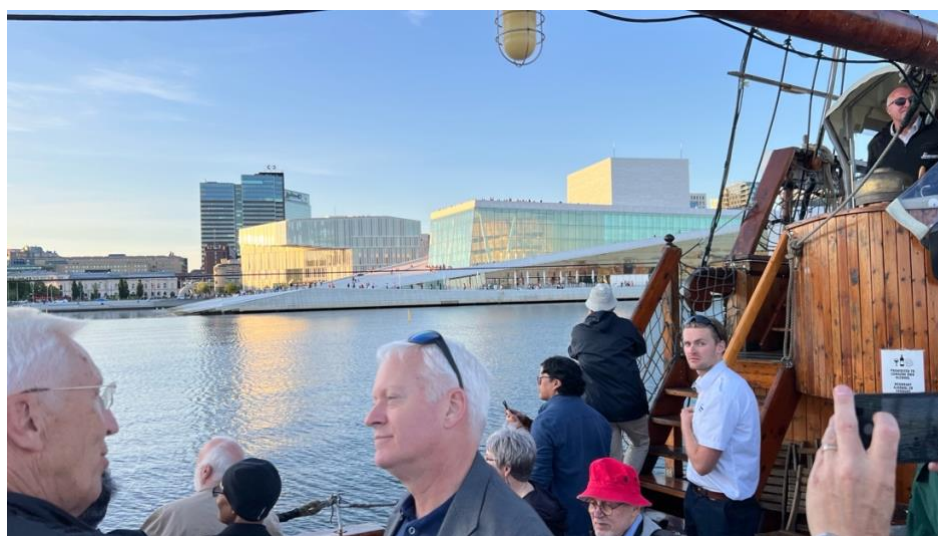
With a total budget on the order of NOK 9.5 million, it was therefore essential to adopt a financial model that avoided these complications. To this end, full financial responsibility for the congress was

assigned to our PCO, acting as a service provider. Gyro Conference handled all participant fees, sponsorship income, supplier contracts, and VAT settlement within its own accounts.

The Hylleraas Centre provided an initial, limited loss guarantee, while the Faculty of Mathematics and Natural Sciences at the University of Oslo guaranteed coverage of any potential additional financial losses. This model proved crucial in making a congress of this scale feasible within the given regulatory framework. Any financial surplus accrues to the Faculty of Mathematic and Natural Sciences.

WATOC Board Meeting and Dinner Cruise

In connection with the congress, the WATOC Board held a board meeting at 3 p.m. on June 21 at the Oslo Congress Centre. The meeting was followed at 7 p.m. by a three-hour dinner cruise on the Oslo Fjord for board members and accompanying persons, in glorious weather. As members of the board, Odile Eisenstein and Trygve Helgaker attended these meetings.



Dinner cruise of WATOC Board on the Oslo Fjord on Saturday. Photo: Trygve Helgaker

Satellite Meetings

Three satellite meetings were held in connection with WATOC 2025 — two before the WATOC congress and one after the congress.

The satellite *Current Trends in Electronic-Structure Theory (CTEST-2025)*, took place at the Carlsberg Academy in Copenhagen from June 18 to 20 with 75 participants. The meeting was organized by Sonia Coriani and Janus Eriksen from the Technical University of Denmark.

The second, *Numerical Methods in Quantum Chemistry*, was held at Humboldt University of Berlin, also on 18–20 June, organized by Florian Bischoff (Humboldt University of Berlin), Luca Frediani, and Michal Repisky (UiT The Arctic University of Norway), with 59 participants.

The third, *Reusable Libraries in Quantum Chemistry*, which took place after the WATOC Congress, was held at the Congress Centre Majvik in Finland from June 29 to July 3, 2025, organized by Dage Sundholm and Susi Lehtola from the University of Helsinki. The meeting was attended by 72 participants.