Plenary sessions WATOC 2025

Sunday June 22

Session P1 Chair: Odile Eisenstein

15:40	Michele Parrinello	ETH Zürich & Istituto Italiano di Tecnologia	927	The weird and wonderful world of catalysis
16:20	Veronique van Speybroeck	Ghent University	829	New avenues in modelling realistic nanoporous materials at operating conditions

Session P2 Chair: Peter Gill

17:30	Frank Neese	Max-Planck-Institut für Kohlenforschung	929	The Bubblepole approximation for large molecular systems
18:10	Jan Martin	Weizmann Institute of Science	954	Accurate thermochemistry, kinetics, and spectroscopy: the high and low roads

Wednesday 25 June

Session P3 Chair: Peter Gill

08:30	Gustavo Scuseria	Rice University	848	Symmetry-projected coupled cluster theory
09:10	Katharina Boguslawski	Nicolaus Copernicus University in Toruń	879	Is simpler better? Alternative wave function approaches for molecular modeling

Session P4 Chair: Martin Head-Gordon

10:20	Luhua Lai	Peking University	851	Computational approaches for making undruggable targets druggable
11:00	Heather Kulik	Massachusetts Institute Of Technology	418	What has machine learning taught us about transition metal chemistry?

Friday 27 June

Session P5 Chair: Peter Gill

08:30	Mario Motta	IBM Research Yorktown	983	Quantum chemistry calculations using classical and quantum computers in concert
09:10	Edit Mátyus	Eötvös Lorand University	934	Molecular quantum dynamics by solving the rovibrational Schrödinger equation

Session P6 Chair: Peter Gill

10:20	Alexander Sokolov	Ohio State University	415	Efficient multireference methods for excited states and spectroscopy
11:00	Thomas Jagau	KU Leuven	939	Recent progress in complex-energy electronic-structure methods