Historical talks (H)

#	Speaker	Institution	Title	Time
H1	Rodney J. Bartlett	U Florida, Gainesville, FL, USA	Per-Olov Löwdin, 1916–2000	Session 2, Tue. 19, 10:45–11:00
H2	Paul W. Ayers	McMaster U, Hamilton, ON, Canada	Robert G. Parr, 1921–2017	Session 4, Wed. 20, 10:45–11:00
H3	Peter M. W. Gill	Australian National U, Canberra, Australia	John Pople: The Man and the Message	Session 6, Thu. 21, 10:45–11:00
H4	Jean-Paul Malrieu	U Paul Sabatier, Toulouse, France	About Raymond Daudel, Alberte and Bernard Pullman, from Hückel Hamiltonians to the Foundation of ICQC	Session 7, Fri. 22, 10:45–11:00

Lectures (L)

#	Speaker	Institution	Title	Time
L1	Walter Thiel	MPI, Mülheim an der Ruhr, Germany	Accuracy versus Complexity in Computational Chemistry	Session 1, Mon. 18, 17:15–17:45
L2	Fernando Martín	U Autónoma Madrid & IMDEA-Nano, Madrid, Spain	Attosecond Pump-Probe Spectroscopy of Aminoacids	Session 1, Mon. 18, 17:45–18:15
L3	Chantal Daniel	CNRS & U Strasbourg, France	Excited States and Coordination Chemistry	Session 1, Mon. 18, 18:15–18:45
L4	Wim Klopper	KIT, Karlsruhe, Germany	Bethe-Salpeter Approach for Molecular Quantum Chemistry	Session 2, Tue. 19, 08:45–09:15
L5	Kristine Pierloot	KU Leuven, Belgium	Recent Studies in Multiconfigurational Transition Metal Chemistry	Session 2, Tue. 19, 09:15–09:45
L6	Koichi Ohno	Tohoku U, Sendai & IQCE, Tokyo, Japan	Global Reaction Route Mapping and Exploration of Novel Chemistry on Potential Energy Surfaces	Session 2, Tue. 19, 09:45–10:15
L7	Wei Wu	Xiamen U, China	Combining Density Functional Theory and Valence Bond Method	Session 2, Tue. 19, 11:00–11:30
L8	Paola Gori-Giorgi	Vrije U Amsterdam, The Netherlands	Fully Non-Local Exchange-Correlation Functionals from the Mathematical Structure of the Strong-Coupling Limit of DFT	Session 2, Tue. 19, 11:30–12:00

L9	Troy Van Voorhis	MIT, Cambridge, MA, USA	Quantum Embedding for Molecular Systems	Session 3, Tue. 19, 14:30–15:00
L10	Sason Shaik	Hebrew U, Jerusalem, Israel	Oriented Electric Fields — New Effectors in Chemistry	Session 3, Tue. 19, 15:00–15:30
L11	Claudia Filippi	U Twente, Enschede, The Netherlands	Efficient Structural and Variational Optimization in Quantum Monte Carlo	Session 3, Tue. 19, 15:30–16:00
L12	Stuart C. Althorpe	U Cambridge, UK	Matsubara Dynamics: Classical Dynamics with Quantum Statistics	Session 3, Tue. 19, 16:30–17:00
L13	Debashree Ghosh	IACS, Kolkata, India	Photo-Processes in Biology – Fast and Accurate Polarizability	Session 3, Tue. 19, 17:00–17:30
L14	Marco Garavelli	U Bologna, Italy	Towards an Accurate Computational Photochemistry and Photobiology: The Paradigmatic Case of Vision	Session 3, Tue. 19, 17:30–18:00
L15	So Hirata	U Illinois, Urbana, IL, USA	One-Particle Many-Body Green's Function Theory: Algebraic Recursive Definitions, Linked- and Irreducible-Diagram Theorems, and General-Order and Stochastic Algorithms	Session 4, Wed. 20, 08:45–09:15
L16	Julien Toulouse	Sorbonne U & CNRS, Paris, France	A General Range-Separated Double-Hybrid Density-Functional Theory	Session 4, Wed. 20, 09:15–09:45
L17	Dominika Zgid	U Michigan, Ann Arbor, MI, USA	Green's Function Methods for Embedding Problems	Session 4, Wed. 20, 09:45–10:15
L18	Pavel Jungwirth	IOCB, Czech Ac. Sci., Prague, Czech Republic	Probing Solvated Electrons by Explosive as well as Non-Explosive Experiments and Simulations	Session 4, Wed. 20, 11:00–11:30
L19	Eva Zurek	U Buffalo, State U New York, NY, USA	Chemistry under Pressure	Session 4, Wed. 20, 11:30–12:00
L20	Katarzyna Pernal	Lodz U Tech, Poland	Correlation Energy for Multireference Ground and Excited States from Adiabatic Connection Approximations	Session 5, Wed. 20, 14:30–15:00

L21	Per E.M. Siegbahn	Stockholm U, Sweden	DFT Modeling of Redox-Active Metalloenzymes	Session 5, Wed. 20, 15:00–15:30
L22	Nicolas Ferré	Aix-Marseille U & CNRS, Marseille, France	How Anabaena Sensory Rhodopsin photochemical properties are tuned by pH	Session 5, Wed. 20, 15:30–16:00
L23	Sonia Coriani	Technical U Denmark, Kongens Lyngby, Denmark	Developing Theoretical Beamlines for Local, Ultrafast and Magnetic-Field Induced Spectroscopic Effects	Session 5, Wed. 20, 16:30–17:00
L24	Ulf Ryde	Lund U, Sweden	Calculating Ligand-Binding Affinities with Quantum-Mechanical Methods	Session 5, Wed. 20, 17:00–17:30
L25	K. Birgitta Whaley	U California, Berkeley, CA, USA	Quantum Computation – the Promise and the Path	Session 5, Wed. 20, 17:30–18:00
L26	Kieron Burke	UC Irvine, CA, USA	Understanding the Successes and Limitations of Density Functionals	Session 6, Thu. 21, 08:45–09:15
L27	Anastassia N. Alexandrova	U California, Los Angeles, CA, USA	Surface-Supported Cluster Catalysis: Fluxionality, Ensembles, and Role of Metastable Sites	Session 6, Thu. 21, 09:15–09:45
L28	Judith Herzfeld	Brandeis U, Waltham, MA, USA	Animating Lewis Dots: Transferrable Sub-Atomistic Force Fields for Efficient, Intuitive, Turnkey Simulations of Chemical Reactions	Session 6, Thu. 21, 09:45–10:15
L29	Feliu Maseras	ICIQ, Tarragona, Spain	Computing the Barrier to Single Electron Transfer in Homogeneous Catalysis	Session 6, Thu. 21, 11:00–11:30
L30	Clemence Corminboeuf	EPFL, Lausanne, Switzerland	Analyzing Non-Covalent Interactions Beyond the Static Picture	Session 6, Thu. 21, 11:30–12:00
L31	Jürgen Gauss	Johannes Gutenberg U, Mainz, Germany	Many-Body Expanded Full Configuration Interaction	Session 7, Fri. 22, 08:45–09:15
L32	Neepa T. Maitra	City U New York, NY, USA	Building Memory-Dependent Functionals for Time-Dependent Density Functional Theory	Session 7, Fri. 22, 09:15–09:45
L33	Fahmi Himo	Stockholm U, Sweden	Recent Developments in the Quantum Chemical Cluster Approach for Enzyme Modeling	Session 7, Fri. 22, 09:45–10:15
L34	Marcel Swart	ICREA, Barcelona & IQCC, Girona, Spain	Decomposing Oxidation Catalysis	Session 7, Fri. 22, 11:00–11:30
L35	Martin Kaupp	Tech U Berlin, Germany	Progress in the Computation and Analysis of Spin-Orbit Effects on Magnetic-Resonance Parameters	Session 7, Fri. 22, 11:30–12:00

L36	Toru Shiozaki	Northwestern U, Evanston, IL, USA	New Frontiers in Multireference Electron Correlation Methods	Session 8, Fri. 22, 14:30–15:00
L37	Georg Kresse	U Vienna, Austria	Self-Energies, Correlation Energies, BSE, and Time-Dependent DFT beyond the Tamm-Dancoff Approximation	Session 8, Fri. 22, 15:00–15:30
L38	Yousung Jung	KAIST, Daejeon, Korea	Small Molecule Activation Using Computational Catalysis and Machine Learning	Session 8, Fri. 22, 15:30–16:00
L39	David P. Tew	MPI, Stuttgart, Germany	Is CCSD(T) any Good for Transition Metal Complexes?	Session 8, Fri. 22, 16:30–17:00
L40	Peter Schwerdtfeger	Massey U Albany, Auckland New Zealand & CAS, Norwegian Ac. Sci. Lett., Oslo, Norway	From the Schrödinger Equation to the Standard Model and Beyond	Session 8, Fri. 22, 17:00–17:30
L41	Markus Reiher	ETH, Zurich, Switzerland	Recent Applications of the DMRG: From Automated Active Orbital Selection to Molecular Vibrations	Session 9, Sat. 23, 08:45–09:15
L42	Zhipan Liu	Fudan U, Shanghai, China	Stochastic Surface Walking (SSW) method for Resolving Global Potential Energy Surface	Session 9, Sat. 23, 09:15–09:45
L43	Attila G. Császár	MTA-ELTE & Eötvös Loránd U, Budapest, Hungary	Astructural Molecules in Motion	Session 9, Sat. 23, 09:45–10:15
L44	Hiromi Nakai	Waseda U, Tokyo, Japan	What is the Best Choice of Embedding-Fragmentation Scheme for Practical Quantum Chemical Simulation?	Session 9, Sat. 23, 10:45–11:15
L45	Trygve Helgaker	CAS & Hylleraas CQMS, Oslo, Norway	Closed-Shell Molecular Paramagnetism from Avoided Crossings	Session 9, Sat. 23, 11:15–11:45