Full Program

		Monday, 09.09.2019	Tuesday, 10.09.2019	Wednesday, 11.09.2019	Thursday, 12.09.2019
09:00	09:40		I4 – BEHLER	I8 – PAVLÍKOVÁ PŘECECHTĚLOVÁ	I11 – CSÁSZÁR
09:40	10:00		C4 – COE	I9 – KUBAS	C17 – SLAVÍČEK
10:00	10:20		C5 – WESTERMAYR		C18 – SULIMAN
10:20	10:50		Coffee break		
10:50	11:30		I5 – PITTNER	I10 – SZABADOS	I12 – DERZSI
11:30	11:50		C6 – FREITAG	C14 – MUSIAŁ	C19 – DARU
11:50	12:10		C7 – HOLZER	C15 – MIHÁLKA	C20 – NAGY
12:10	12:30		C8 – KELTERER	C16 – PRZYBYTEK	C21 – HRIVNÁK
12:30	14:00		Lunch	Lunch	Lunch/ Departure
14:00	14:20	Registration	I6 – BICZYSKO	Excursion	
14:20	14:40				
14:40	14:50		C9 – MONARI		
14:50	15:00	Welcome & Introduction			
15:00	15:20	I1 – REIHER	C10 – TÓTH		
15:20	15:40		Coffee break		
15:40	15:50	I2 – KREWALD			
15:50	16:00		I7 – KOMOROVSKY		
16:00	16:20				
16:20	16:30	Coffee break			
16:30	16:50		C11 – ONČÁK		
16:50	17:10	I3 – GRUDEN	C12 – CVITAŠ		
17:10	17:30		C13 – ESSEFFAR		
17:30	17:50	C1 – ROZGONYI	BM		
17:50	18:10	C2 – BENEDEK			
18:10	18:30	C3 – RYBICKI			
18:30	20:00	Dinner	Dinner		
20:00	22:00	PS I	PS II	Conference Dinner	

I … Invited Speaker

C … Contributed talk

PS … Poster session

BM … Board Meeting

Monday, 9. September

14:00		**Registration**
14:50		**Welcome & Introduction**
15:00		Session 1 - Chair: Leticia González
15:00	I1	**Markus Reiher** – ETH Zürich *Matrix product states for electronic and vibrational structure*
15:40	I2	**Vera Krewald** – Technical University Darmstadt *Orbital entanglement analysis of magnetically coupled transition metal complexes*
16:20		**Coffee break**
16:50		Session 2 - Chair: Szalay Péter
16:50	I3	**Maja Gruden-Pavlović** – University of Belgrade *Spinning around in transition metal chemistry*
17:30	C1	**Tamás Rozgonyi** – Hungarian Academy of Sciences *Studying ultrafast photorelaxation in functional Fe(II) complexes*
17:50	C2	**Zsolt Benedek** – Budapest University of Technology and Economics *Exploring the mechanism of biomimetic nitrogen fixation and its side reactions*
18:10	C3	**Marcin Rybicki** – Humboldt-Universität zu Berlin *Ab initio description of heterogeneous catalysis - monomolecular alkane cracking over H-MFI zeolite*
18:30		**Dinner**
20:00		**Poster Session I: P01 - P35**

Tuesday, 10. September

09:00		Session 3 - Chair: Philipp Marquetand
09:00	I4	**Jörg Behler** – University of Göttingen *Understanding complex systems with high-dimensional neural network potentials*
09:40	C4	**Jeremy Coe** – Heriot-Watt University *Potential energy curves using machine learning configuration interaction*
10:00	C5	**Julia Westermayr** – University of Vienna *Machine learning for excited state dynamics: fitting multidimensional potentials for energies, forces and couplings*
10:20		**Coffee break**
10:50		Session 4 - Chair: Doslic Nadja
10:50	I5	**Jiří Pittner** – Academy of Sciences of the Czech Republic *Molecular dynamics with non-adiabatic and spin-orbit effects*
11:30	C6	**Leon Freitag** – ETH Zürich *Towards ab-initio surface-hopping dynamics with a density matrix renormalization group self-consistent field approach*
11:50	C7	**Christof Holzer** – Karlsruhe Institute of Technology *Prediction of excited state properties for sizable molecular systems including spin-orbit effects*
12:10	C8	**Anne-Marie Kelterer** – Graz University of Technology *The Förster energy transfer in metal organic frameworks*
12:30		**Lunch**

Tuesday, 10. September

14:00		Session 5 - Chair: Jin Wen
14:00	I6	**Malgorzata Biczysko** – Shanghai University *The role of anharmonic corrections in conformational analysis of flexible molecules*
14:40	C9	**Antonio Monari** – Université de Lorraine Nancy *A song of light and life. From molecular modeling to in-silico photobiology*
15:00	C10	**Zsuzsanna Tóth** – University of Chemistry and Technology Prague *Calculating ionization energy in condensed phase using a QM:QM method*
15:20		**Coffee break**
15:50		Session 6 - Chair: Bogumil Jeziorski
15:50	I7	**Stanislav Komorovsky** – Slovak Academy of Science *Relativistic theory for prediction of excitation energies of both closed- and open-shell species*
16:30	C11	**Milan Oncák** – University of Innsbruck *Photochemistry in helium droplets: state-dependent solvation effects in* $Cs_2He_n^+$
16:50	C12	**Marko Tomislav Cvitaš** – Ruđer Bošković Institute *Tunnelling splittings in water clusters using instantons*
17:10	C13	**M'hamed Esseffar** – Cadi Ayyad University *Diastereoselective synthesis and cytotoxic evaluation of new isoxazoles and pyrazoles with monoterpenic skeleton.*
17:30		**Board Meeting**
18:30		**Dinner**
20:00		**Poster Session II: P36 - P70**

Wednesday, 11. September

09:00		Session 7 - Chair: A. Daniel Boese
09:00	I8	**Jana Pavlíková Přecechtělová** – Central European Institute of Technology-Czech Republic *Computation of NMR chemical shifts in phosphorylated intrinsically disordered proteins: challenges and limitations*
09:40	I9	**Adam Kubas** – Polish Academy of Sciences *Mechanistic insights into Z-selectivity in (photo)catalytic retinoid synthesis*
10:20		**Coffee break**
10:50		Session 8 - Chair: Jozef Noga
10:50	I10	**Ágnes Szabados** – Eötvös Loránd University *Ring Coupled Cluster Doubles at the Multireference Level*
11:30	C14	**Monika Musiał** – University of Silesia in Katiwice *Intruder-free Fock space multireference coupled cluster method in the molecular studies*
11:50	C15	**Zsuzsanna Mihálka** – Eötvös Loránd University *Half-projection applied to the strongly orthogonal geminal product wavefunction*
12:10	C16	**Michal Przybytek** – University of Warsaw *Dispersion energy of symmetry-adapted perturbation theory from the explicitly correlated F12 approach*
12:30		**Lunch**
14:00		**Free afternoon**
19:30		**Get together**
20:00		**Conference dinner**

Thursday, 12. September

09:00		Session 9 - Chair: Miroslav Iliaš
09:00	I11	**Attila Császár** – Eötvös Loránd University *Quasistructural molecules*
09:40	C17	**Petr Slavíček** – University of Chemistry and Technology Prague *The concept of error in computational spectroscopy*
10:00	C18	**Siba Suliman** – Comenius University *Microhydration of HOIO: structural and thermochemical properties of HOIO + n H_2O (n = 1 -4)*
10:20		**Coffee break**
10:50		Session 10 - Chair: Peter Surjan
10:50	I12	**Mariana Derzsi** – Slovak University of Technology *Exploring crystal chemistry of silver(II) with DFT modelling*
11:30	C19	**Janos Daru** – Ruhr-Universität Bochum *Restricting solvation to two dimensions: soft landing of microsolvated ions on inert surfaces*
11:50	C20	**Tibor Nagy** – Hungarian Academy of Sciences *A novel, thermodynamics-based objective function for the parameterization of molecular mechanics force fields*
12:10	C21	**Tomáš Hrivnák** – Comenius University *The rigorous local field approach for the effective calculation of linear and nonlinear optical properties of solvated systems*
12:30		**Lunch / Departure**

P01 **Alonso Gil Santiago** - Czech Academy of Sciences
SAM radical decay in solution vs. in PFL-AE/LAM enzymatic environment

P02 **Antalik Andrej** - Czech Academy of Sciences
The peculiar case of oxo-Mn(Salen)

P03 **Antusek Andrej** - Slovak University of Technology
NMR shielding in transition metal complexes and nuclear magnetic dipole moments of stable transition metal nuclei

P04 **Boese Daniel** - University of Graz
Molecular Crystals of Tetra-Ethenyl-group(XIV) Compounds

P05 **Brandejs Jan** - Charles University
Relativistic coupled clusters externally corrected by four-component DMRG

P06 **Breza Martin** - Slovak Technical University
On shape dependence of rutile nanoparticles toxicity

P07 **Bucinsky Lukas** - Slovak Technical University
How to teach a non-relativistic wavefunction relativity

P08 **Cagardova Denisa** - Slovak University of Technology in Bratislava
New Generations of Sunflower Molecules: Theoretical Study of Electronic Structure and Charge Transport

P09 **Carsky Petr** - Academy of Sciences of the Czech Republic
Prospects of using mixed Gaussian and plane wave basis sets and graphics processing units in mainstream quantum chemistry

P10 **Cosic Rajko** - Technical University of Ostrava
Calculations of the Photoabsorption Spectra of Small Charged Helium Clusters

P11 **Demel Ondrej** - Czech Academy of Sciences
Laplace MP2 method with mixed Gaussian / Plane wave Density Fitting

P12 **Dinu Dennis** - LFU Innsbruck
On the Synergy of Matrix-Isolation Infrared Spectroscopy and Vibrational Configuration Interaction Computations

P13 **Dolgonos Grygoriy** - University of Graz
Improving the benchmark data for the lattice volumes and energies of X23 molecular crystals

P14 **Fanta Roman** - University of Ostrava
Toward Accurate Noncovalent Interactions by Scalable Quantum Monte Carlo

P15 **Farcas Alex Adrian** - "Babeş-Bolyai" University
The influence of the metal-ligand charge transfer effects on the structural stability and the strength of the spin-orbit coupling in Ni(II)-based metal-ligand complexes

P16 **Feyersinger Florian** - University of Graz
Density Embedding for Organic Molecules on Surfaces

P17 **Girnt Peter** - Budapest University of Technology and Economics
Estrogen-quinone-induced DNA modifications: A computational study

P18 **Grabowska Ewelina** - Nicolaus Copernicus University
A new adiabatic method of averaging intermolecular interaction energy over vibrations of the monomers.

P19 **Granatier Jaroslav** - Slovak University of Technology
The extrapolation Atomic Natural Orbitals of basis set to complete basis set (CBS) limit

P20 **Guttmann Robin** - University of Graz
High-accurate Geometries and Intermolecular Interaction Energies of small Systems

P21 **Hoja Johannes** - University of Graz
Accuracy of Density-Functional Approximations and QM:QM Embedding Methods for Molecular Crystals

P22 **Ilias Miroslav** - Matej Bel University
Electronic structure, bonding and volatility of carbonyl compounds of Tc, Re, and Bh

P23 **Kellö Vladimir** - Comenius University in Bratislava
Electronic excited states of AuSi

P24 **Kozakova Silvia** - Comenius University in Bratislava
Spectroscopic properties of diatomic molecules CdI and CsCd

P25 **Kozma Balazs** - ELTE Eötvös Loránd University
Benchmark calculations with Coupled Cluster methods on Charge Transfer

P26 **Kuroki Nahoko** - Chuo University
Electronic Structure Informatics for Exploring Efficient CO 2 Adsorbents

P27 **Lesiuk Michal** - University of Warsaw
Implementation of the full CCSDT method with tensor decompositions

P28 **Mai Sebastian** - Vienna University of Technology
Comparison of Ultrafast Intersystem Crossing in Iron(II) and Rhenium(I) Complexes

P29 **Malcek Michal** - Slovak University of Technology
Binuclear Cu-Cu/Cr-Cr paddle wheel complexes: Theoretical study

P30 **Margocsy Adam** - Eötvös Loránd University
Application of the GVB-rCCD method to simple molecular systems

P31 **Marquetand Philipp** - University of Vienna
Machine learning for dynamics simulations

P32 **Matousek Mikulas** - ASCR
Lowest Spin States Energetics in Fe(II)-Porphyrin Model

P33 **Medved Miroslav** - Matej Bel University
The ups and downs of DFT in high-order electric property calculations for hydrogen-bonded systems

P34 **Mitic Marco** - University of Belgrade
Vibronic and spin-orbit coupling in the X $^2\Pi_u$ state of $SCCS^-$: An ab initio approach

P35 **Modrzejewski Marcin** - Charles University
Random phase approximation for many body noncovalent systems

P36 **Mori Hirotoshi** - Chuo University
Ultrafast Quantum Chemical Screening of Azeotropic Mixture

P37 **Mrovec Martin** - Technical University of Ostrava
An Optimization Approach to Solving the Kohn-Sham Equation

P38 **Papp Marcell** - Budapest University of Technology and Economics
Exploring Hydrogen Amplification Reaction and Deactivation Mechanism of Biomimetic Fe-nitrogenases

P39 **Papp Mariann** -
Investigation of electronic spin states in substituted $[Fe(terpy)_2]^{2+}$ *functional molecules*

P40 **Pasteka Lukas** - Comenius University
Bullvalene, a molecular shape shifter

P41 **Pitesa Tomislav** - Ruđer Bošković Institute
Anti-Kasha nitrogen photoelimination from diazoalkanes

P42 **Pluta Tadeusz** - University of Silesia
Determination of dynamic higher-order electric response properties. Mixed analytical/numerical approach

P43 **Ponzi Aurora** - Ruđer Bošković University
Multi-slit-type interference in C 2s photoionization of polyatomic molecules

P44 **Puskarova Ingrid** - Slovak University of Technology
The electronic structure of the transition metal complexes

P45 **Rozza Ahmed** - Budapest University of Technology and Economics
Mapping Pathways of Diatomic Ligand Migration into H-NOX Domains as a Modelof SGC Activation

P46 **Rutkowska Zbik-Dorota** - Polish Academy of Sciences
Catalytic properties of vanadium centers introduced into BEA zeolite

P47 **Sagan Filip** - Jagiellonian University
An Extension of the Charge and Energy Decomposition Scheme (ETS-NOCV) – On the Importance of Kinetic and Potential Energy Contributions in Chemical Bonding

P48 **Said Halima** - Comenius University in Bratislava
Structure and electronic properties of clean and wet Cs(001)

P49 **Sapunar Marin** - Ruđer Bošković Institute
Wave function overlap based assignment of UV absorption spectra and state specific analysis of solvation effects

P50 **Schwiedrzig Ludwig** - University of Vienna
Shine a Light on Me: Simulating the Reactivity of a Water Oxidation Catalyst

P51 **Semrad Hugo** - Masaryk University
Reaction Energetics & Diels-Alder Reaction Profiles for Enediones and Decalines by Means of DFT

P52 **Siecinska Sylwia** - Nicolaus Copernicus University
The kinetic energy potential from Kohn-Sham non-interacting kinetic energy expression.

P53 **Skrzynski Grzegorz** - University of Silesia
Electric properties of carbazole and its derivatives

P54 **Sochorova Vokacova Zsuzsana** - Academy of Sciences of the Czech Republic
Simulation of organic solvents and their effect on Candida antarctica lipase B

P55 **Srsen Stepan** - University of Chemistry and Technology
Electronicspectra beyond the nuclear ensemble method

P56 **Steklac Marek** - Slovak University of Technology
Quantumchemical study of ortho-quinones toxicity through their copper(II) coordination ability

P57 **Sulka Martin** - Slovak University of Technology in Bratislava
Fragmentation of NOON-based measures for assessing the expected bias cancellation in SD FNDMC.

P58 **Tucholska Aleksandra** - University of Warsaw
Lifetimes of alkaline earth atoms computed within the Hermitian formulation of the coupled cluster response theory

P59 **Tulipan Levente** - ELTE Eötvös Loránd University
The effect of Spin-Component-Scaling on excited state CC2 and ADC(2) potential energy surfaces

P60 **Urban Miroslav** - Comenius University
CCSD(T) benchmark calculations and DFT modeling of polyethylene crosslinked by metallic atoms

P61 **Venosova Barbora** - Slovak University of Technology
Study of electronic structure and CO 2 affinity of complexes of transition metals

P62 **Wasif Baig Mirza** - Czech Academy of Sciences
Theoretical investigation of effect of alkylation and bromination on spin-orbit couplings in BODIPY based photosensitizers

P63 **Wen Jin** - University of Vienna
Searching for Optimal Arrangements of Perylene Pairs in Singlet Fission