Sunday

14:00	**Registration**	
15:50	**Opening**	

Session I

Bogumil Jeziorski

16:00	**Martin Krupicka**	Mechanochemical indicators
16:40	**Simon Budzak**	Excited state properties as a key to understand molecular probes
17:20	**Dana Nachtigallova**	Excited states of polycyclic aromatic systems
17:40	**Marin Sapunar**	Computation of many-electron wave function overlaps for photochemical studies

18:00	**Dinner**
20:00	**Poster Session A**

Monday_AM

Session II Miroslav Urban		
08:20	**Michal Repisky**	All-electron fully relativistic KS theory for solids based on the Dirac–Coulomb Hamiltonian and Gaussian-type functions
09:00	**Leticia González**	Excited state dynamics of transition metal complexes
09:40	**Lukáš Félix Pašteka**	Reuniting theory and experiment, the case study on gold
10:00	**Paweł Tecmer**	Unconventional electronic structure methods in actinide chemistry
10:20	**Coffee Break**	
Session III Peter Surjan		
10:50	**Jiri Klimes**	Towards an accurate theoretical description of molecular solids
11:30	**Ctirad Červinka**	Towards reasonable ab initio sublimation pressures for molecular crystals
11:50	**Oleksandr Loboda**	Fragment-based DFT methods for molecular crystals
12:10	**Lunch**	

Monday_PM

Session IV

Leticia Gonzáles

14:00	**Alexandre Tkatchenko**	The promise and rise of machine learning in chemistry and physics
14:40	**Peter Poliak**	Thermodynamics of radical scavenging activity of selected carotenoids
15:00	**Mario Vazdar**	Arginine “magic”: Guanidinium like-charge ion pairing from aqueous salts to cell penetrating peptides
15:20	**Miroslav Rubes**	Theoretical description of CO adsorption in H-FER zeolite
15:40	**Coffee Break**	

Session V

Miroslav Medveď

16:10	**Michal Lesiuk**	Approximate coupled-cluster schemes with singular-value decomposition of the triple excitations amplitudes
16:50	**Tatiana Korona**	Energy and density partitioning as tools for investigations of intermolecular complexes - several case studies
17:10	**Szymon Śmiga**	Approximate solution of CC equations: Application to the CCD method and non-covalent interacting systems
17:30	**Ágnes Szabados**	Geminal PT based on the UHF wavefunction
17:50	**Jan Novotny**	Interpreting NMR parameters of metal complexes using relativistic DFT calculations
18:10	**Dinner**	
20:00	**Poster Session B**	

Tuesday

Session VI

Stanisław Kucharski

08:20	**Tamás Szidarovszky**	Rovibronic spectra of light-dressed molecules
09:00	**Georg Madsen**	Phonon superscatterers
09:40	**Aurora Ponzi**	Study of dynamical observables involved in photoionization process
10:00	**Ivan Černušák**	Raman spectroscopic study of polysulfanes in natural fluid inclusions
10:20	**Coffee Break**	

Session VII

Jiri Pittner

10:50	**Örs Legeza**	Coupled-cluster method tailored by tensor-network states in quantum chemistry
11:30	**Katharina Boguslawski**	Tailored coupled cluster approaches to model strong correlation across the periodic table
11:50	**Ádám Margócsy**	Multiple bond breaking with APSG based correlation methods
12:10	**Lunch**	
13:30	**Excursion**	
18:30	**Conference Dinner**	

Wednesday

Session VIII

Anne-Marie Kelterer

08:40	**Robert Izsak**	Wave function methods for excited states and spectroscopic applications
09:20	**Robert Zalesny**	Nonempirical simulations of two-photon electronic absorption spectra of molecules in solution
10:00	**Stefan Varga**	Infinite lattice sums with Bloch phase factors
10:20	**Coffee Break**	

Session IX

Péter G. Szalay

10:50	**Dmitry Fedorov**	A new point of view on the van der Waals radius
11:10	**Michal Malček**	Theoretical study of Ru- and Mn-based coordination compounds with biological activity
11:30	**Ivana Niksic-Franjic**	Mechanisms and kinetics of charge transfer processes in aqueous reactions of free radicals
11:50	**Closing**	
12:00	**Lunch & Departure**	

List of Posters

Session A

A1	**Andrej Antalík**	Local pair natural orbital coupled clusters tailored by matrix product states
A2	**Andrej Antusek**	Nuclear magnetic moment of 209Bi from new NMR experiments
A3	**Tarek Ayari**	Theoretical and dynamic study of malonaldehyde
A4	**Maria Barysz**	
A5	**A. Daniel Boese**	ZMP-SAPT: DFT-SAPT using ab initio densities
A6	**Jiri Brabec**	Domain-based local pair natural orbital version of Mukherjee's state-specific coupled cluster method
A7	**Jan Brandejs**	Hilbert space multireference coupled clusters tailored by matrix product states
A8	**Martin Breza**	On the Al=Al double bond in the $LiAl_2H_4^-$ cluster
A9	**Zlatko Brkljača**	Calculations of pK_a value of lysine in biological membranes
A10	**Marek Štekláč**	Model study of the anticancer drug camptothecin
A11	**Denisa Cagardová**	DFT study of the effect of chemical modification on the electronic structure and drift mobilities of selected pentacene and bis-benzothiadiazole derivatives
A12	**Grygoriy Dolgonos**	Adjusting dispersion coefficients for the accurate DFTB+D3 treatment of structural and energetic properties of molecular crystals
A13	**Nađa Došlić**	Is visible fluorescence in non-aromatic peptidic chains possible?
A14	**Matus Dubecky**	Gaussian basis set saturation in fixed-node diffusion Monte Carlo
A15	**Philippe Durand**	Tilde transformation for quantum resonances
A16	**Roman Fanta**	Benchmark computations of infinite linear chain of HF molecules
A17	**Ewelina Grabowska**	Theoretical spectra of the HD-CO complex to guide the microwave measurements

Session A

A18	**Ireneusz Grabowski**	Practical, accurate, cost- and implementation-free method (ΔMP2-SCS(IP)) for the calculation of vertical ionization potentials
A19	**Jaroslav Granatier**	Benchmark CCSD(T)/CBS interaction energies of coinage metal atoms on benzene
A20	**Peter Grancic**	Molecular modelling of bioorganoclays
A21	**Robin Guttmann**	HB49: How accurate is DFT?
A22	**Tomáš Hrivnák**	Interaction-induced electric properties of hydrated uracil molecule
A23	**Michał Chojecki**	Chiral resolution of the active pharmaceutical intermediates on the selected stationary phases
A24	**Miroslav Iliaš**	Theoretical study of molecular and adsorption properties of group 6, 7 and 8 heavy and super-heavy metal carbonyls
A25	**Katarzyna Jakubowska**	Relativistic four component DFT and CC calculations of potential energy curves of Zn_2, Cd_2 and Hg_2 dimers
A26	**Wojciech Jankiewicz**	Failure of the dispersion-corrected density-functional theory for three-body intermolecular interactions.
A27	**Frantisek Karlicky**	Fluorographane C_2FH: stable and wide band gap insulator with huge excitonic effect
A28	**Vladimír Kellö**	Calculations of electronic excited states of CsMo molecule
A29	**Anne-Marie Kelterer**	Theoretical Study on Fe(III) and Cu(II) complexes of 4-Quinazolinone in Water and DMF
A30	**Miroslav Kolos**	Adsorption of trichloroethylene on modified zero-valent nanoparticles of iron
A31	**Lukas Konecny**	Relativistic two- and four-component electron dynamics approach to chiroptical spectroscopies

Session B

B1	**Magdalena Krzuś**	DFTB parametrization for intermolecular interactions
B2	**Martyna Krzyżowska**	Two- and three-body interaction energies from DLPNO-CCSD(T)
B3	**Aleksandra Lachmanska**	New theoretical approaches for strongly-correlated systems
B4	**Jakub Lang**	Pertuberative triples correction to DLPNO-MkCCSD
B5	**Pengbo Lyu**	Theoretical investigation of COF stacking and effects on photocatalysis
B6	**Katarzyna Madajczyk**	Benchmarking database for open shell systems
B7	**Ján Matúška**	Formation of tungsten clusters
B8	**Miroslav Medveď**	Photoswitching mechanism of donor-acceptor Stenhouse adducts (DASAs): Theoretical aspects
B9	**Martin Michalík**	Theoretical prediction of electronic structure and drift mobilities of organic semiconductors
B10	**Eva Zsuzsanna Mihalka**	Convergence issues in Rayleigh-Schrodinger perturbation theory: The inverse boundary value problem
B11	**Wasif Baig Mirza**	Quantum chemical study of intersystem crossing between singlets and triplets of 6,7-dibromo-2-ethyl-1,3-dimethyl-4,4-difluoro-4-bora-3a,4a-diaza-s-indacene
B12	**Eva Muchova**	Electronic structure of electrolyte solutions
B13	**Artur Nowak**	Dissecting electron correlation effects in geminal-based wave function method
B14	**Ivana Paidarová**	The state-selected reactions of electronically excited oxygen ions with methane: the role of the spontaneous emission at the long distance region.
B15	**Tadeusz Pluta**	Dynamic polarizability of the tiophene dimer
B16	**Kyrylo Prokofiev**	Towards accurate calculations of adsorption energies
B17	**Ingrid Puškárová**	The electronic structure, UV/Vis transitions and CO_2 affinity of Ni(II)L macrocyclic complexes
B18	**Dorota Rutkowska-Zbik**	DFT modelling of V-containing BEA zeolite

Session B

B19	**Hugo Semrád**	A quantum chemical study of the isomerization steps within acetylene bromoboration
B20	**Jan Simunek**	Thermochemical hierarchy of homodesmotic reactions extended for hydrocarbons containing heteroatoms
B21	**Zuzana Sochorová Vokáčová**	Enzyme activity of Candida antarctica lipase B in organic solvents
B22	**Marcin Stachowiak**	Theoretical studies on ground state and excited states of the NaLi molecule
B23	**Jakub Stošek**	Quantum chemical studies of acetylene bromoboration
B24	**Siba Suliman**	Reaction of CH_2IOH with OH radical
B25	**Mateusz Szczygieł**	Theoretical description of the photoionization process
B26	**Sonia Taamali**	Thermochemistry of HIO_2 species and reactivity of iodous acid with chlorine atom: A computational approach
B27	**Michal Tarana**	Electron-molecule scattering in context of long-range Rydberg molecules
B28	**Miroslav Urban**	Crosslinking in polyethylene by Au and dispersion attractions
B29	**Barbora Venosova**	A comparison of theoretical and experimental electron structures. A N-O bond precedence in 3-alkoxy-4-methylthiazole- 2(3H)-thione derivatives
B30	**Jin Wen**	An MS-CASPT2 calculation of the excited electronic states of an axial BODIPY dimer
B31	**Roman Witasek**	Interactions between dodecamers of hyaluronan and hyaluronan-like molecules with TSG-6 protein
A32	**Libor Veis**	Variational quantum algorithms for strongly correlated quantum chemistry