18th Central European Symposium on Theoretical Chemistry 2022
7th - 10th September, 2022
SDG Family Hotel & Conference Center

Programme

September 7th (Wednesday)

9:00 - Arrival and registration

13:20 - 13:30 Opening

Chair: Péter G. Szalay

Invited Lectures

13:30 - 14:00 **Olga Malkina** - *Institute of Inorganic Chemistry, Slovak Academy of Sciences, Slovakia*
A mystery of a through-space indirect NMR spin-spin coupling between two hydrogen atoms

14:00 - 14:30 **Zdenek Futera, Outi Vilhelmiina Kontkanen, Denys Biriukov** - *Faculty of Science, University of South Bohemia, Czech Republic*
Electron transport on biomolecular interfaces with metal electrodes

Oral Lecture

14:30 - 14:50 **Michał Lesiuk** - *Faculty of Chemistry, University of Warsaw, Poland*
High-level coupled-cluster methods with tensor decomposition

14:50 - 15:10 Coffee break

Chair: Jozef Noga

Invited Lecture

15:10 - 15:40 **Radu Silaghi-Dumitrescu** - *Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, Cluj-Napoca, Romania*
Spectral simulations for bioinorganic centers: in the eye of the beholder

Oral Lectures

15:40 - 16:00 **Matej Uhliar; Denisa Mastiľák Cagardová; Ján Matúška** - *Department of Chemical Physics, Slovak University of Technology in Bratislava, Slovakia*
On aromaticity and electronic properties of selected organic molecules: a theoretical study of relation between the two

16:00 - 16:20 **Michael Bakker; Jana Pavlikova; Amina Gaffour** - *Charles University, Hradec Kralove, Czech Republic*
Probing disordered proteins' phase space of NMR chemical shifts with fragmentation and machine learning

16:20 - 16:40 **Katarzyna Jakubowska; Magdalena Pecul; Kenneth Ruud** - *Faculty of Chemistry, University of Warsaw, Poland*
Vibrational corrections to NMR spin-spin coupling constants from relativistic four-component DFT calculations

16:40 - 17:00 Coffee break

Chair: Nađa Došlić

Invited Lecture

17:00 - 17:30 **Bence Balázs Mészáros; János Daru** - *ELTE Eötvös Loránd University, Hungary*
Pushing mechanistic studies to the limits. But in which direction?

Oral Lectures

17:30 - 17:50 **Péter Pál Fehér, Ádám Madarász, András Stirling** - *Research Centre for Natural Sciences, Hungary*
Benchmarking computational approaches for the prediction of molecular properties pivotal in photocatalysis

17:50 - 18:10 **Dóra Vörös, Andrea Angeletti, Cesare Franchini, Sebastian Mai, Leticia González** - *Institute for Theoretical Chemistry, Faculty of Chemistry, University of Vienna, Austria*
Adsorption and photochemistry of a functionalized push-pull stilbene

18:10 - 18:30 **Mihael Eraković; Marko T. Cvitaš** - *Ruđer Bošković Institute, Croatia*
Instanton approach for simulation of vibration-rotation-tunneling spectra of multi-well systems

18:30 - 19:30 Supper

19:30 - Poster section I.

September 8th (Thursday)

Chair: Jiří Pittner

Invited Lecture

09:00 - 09:30 **Robert W. Góra** - *Faculty of Chemistry, Wroclaw University of Science and Technology, Poland*
Photochemical origins of life elucidated by *ab initio* quantum chemistry

Oral Lectures

09:30 - 09:50 **Tomislav Piteša, Marin Sapunar, Nađa Došlić** - *Ruđer Bošković Institute, Croatia*
Diabatization of electronic states along nonadiabatic trajectories

09:50 - 10:10 **Michał Hapka; Michał Przybytek; Katarzyna Pernal** - *Faculty of Chemistry, University of Warsaw, Poland*
Symmetry-adapted perturbation theory based on multiconfigurational wave function description of monomers

10:10 - 10:50 Coffee break

Chair: Miroslav Medved

Invited Lecture

10:50 - 11:20 **Lukas Bucinsky; Michal Malček; Martin Breza; Joshua Telser** - *Slovak University of Technology, Bratislava Slovakia*
Electronic structure of $[M(N{=}CMe_2)_4]$ complexes

Oral Lectures

11:20 - 11:40 **Péter Jeszenszki; Dávid Ferenc; Edit Mátyus** - *ELTE Eötvös Loránd University, Hungary*
Variational Dirac–Coulomb approach with explicitly correlated basis functions

11:40 - 12:00 **Michał Przybytek** - *Faculty of Chemistry, University of Warsaw, Poland*
He_3 interaction potential: asymptotic behavior of the post-Born-Oppenheimer corrections

12:00 - 13:30 Lunch

13:30 - 18:30 Free

18:30 - 19:30 Supper

19:30 - Poster section II.

September 9th (Friday)

Chair: Géza Fogarasi

Invited Lecture

09:00 - 09:30 **Antonio Prlj; Basile F. E. Curchod** - *University of Bristol, United Kingdom*
Investigating sunlight-triggered excited-state dynamics of transient atmospheric molecules

Oral Lectures

09:30 - 09:50 **Michal Belina; Petr Slavíček; Kirsten Andrea Schnorr** - *University of Chemistry and Technology, Department of Physical Chemistry, Czech Republic*
Direct observation of the fastest acid-based reactions: combining FEL experiments with *ab initio* theory

09:50 - 10:10 **Anna Grabarz; Borys Ośmiałowski** - *Faculty of Chemistry, Wroclaw University of Science and Technology, Poland*
Application of modern density functionals in modeling of excited states of organic dyes

10:10 - 10:50 Coffee break

Chair: A. Daniel Boese

Invited Lecture

10:50 - 11:20 **Sourav Pal** - *Indian Institute of Science Education and Research Kolkata; Visiting Professor, Ashoka University, Sonipat, Haryana, India*
Complex absorbing potential based coupled cluster method for resonance and decay

Oral Lectures

11:20 - 11:40 **Gabriel Rath, Wassja A. Kopp, Kai Leonhard** - *Institute of Technical Thermodynamics, RWTH Aachen University, Germany*
Accurate anharmonic partition functions using low-cost Hamiltonians and Monte Carlo Integration

11:40 - 12:00 **Julianna Oláh; Zsolt Benedek; Marcell Papp; Joseph Kfoury; Tibor Szilvási** - *Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Hungary*
The mechanism of biomimetic nitrogen fixation: insights from quantum chemistry and microkinetic modelling

12:00 - 13:30 Lunch

Chair: Pavel Neogrády

Invited Lectures

13:30 - 14:00 **Joanna Jankowska** - *Faculty of Chemistry, University of Warsaw, Poland*
To infinity, and beyond: expanding the *on-the-fly* NAMD capabilities for modeling cutting-edge photophysical phenomena

14:00 - 14:30 **Alexandru Lupan, Amr A. Attia, Szabolcs Jákó, Attila-Zsolt Kun, R. Bruce King** - *Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, Romania*
Unusual non-spherical deltahedra in metallaborane structures

Oral Lecture

14:30 - 14:50 **Jakub Lang; Michal Przybytek; Michal Lesiuk; Bogumil Jeziorski** - *Faculty of Chemistry, University of Warsaw, Poland*
Ab initio study of three-body polarizability of helium

14:50 - 15:10 Coffee break

Chair: Robert W. Góra

Invited Lecture

15:10 - 15:40 **Tomica Hrenar** - *Department of Chemistry, University of Zagreb Faculty of Science, Croatia*
Building potential energy surfaces *on-the-fly* by deep learning

Oral Lectures

15:40 - 16:00 **Piotr Wróbel; Piotr Kubisiak; Andrzej Eilmes** - *Faculty of Chemistry, Jagiellonian University in Cracow*
AIMD simulations in modelling IR spectra of liquids

16:00 - 16:20 **D. Mišenková; F. Lemken; M. Repiský; J. Noga; O. L. Malkina; S. Komorovský** - *Institute of Inorg. Chem., Slovak Academy of Sciences, Slovakia*
Overcoming the gauge problem for g-tensor calculations in the framework of four-component DFT

16:20 - 16:40 **Milan Ončák; Magdalena Salzburger; Gabriel Schöpfer; Christian van der Linde; Ethan Cunningham; Martin K. Beyer** - *Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria*
Master Equation Modeling of Black Body Infrared Radiative Dissociation

16:40 - 17:00 Coffee break

Chair: Péter Surján

Invited Lecture

17:00 - 17:30 **Paul G. Mezey** - *Kyoto University, Japan; Eötvös Loránd University, Hungary*
Bonding Between Molecular Fragments Shows the Flaws of Persistent Pre-Quantum Chemistry Models

Oral Lectures

17:30 - 17:50 **Dennis F. Dinu; Martin Tschöpe; Benjamin Schröder; Klaus R. Liedl; Guntram Rauhut** - *Deparment of General, Inorganic and Theoretical Chemistry, University of Innsbruck, Austria; Institute for Theoretical Chemistry, University of Stuttgart, Germany*
Spectroscopic constants from rovibrational configuration interaction calculations

17:50 - 18:10 **Michal Malček; Lukáš Bučinský** - *Institute of Physical Chemistry and Chemical Physics, Slovak University of Technology, Slovakia*
Modified graphene quantum dots as hydrogen storage devices

18:10 - 18:30 **Valera Veryazov** - *Theoretical Chemicstry, Lund University, Sweden*
How to apply multiconfigurational theory to ionic solids?

18:30 - 18:50 **József Csóka** - *Department of Physical Chemistry and Materials Science, Faculty of Chemical Technology and Biotechnology, Budapest University of Technology and Economics, Hungary*
Analytic gradients for local density fitting Hartree-Fock and Kohn-Sham methods

19:00 - Conference dinner

September 10th (Saturday)

Chair: Tomica Hrenar

Invited Lecture

09:00 - 09:30 **Ctirad Červinka; Petr Touš** - *Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czechia*
Anisotropy, local disorder and polymorphism of molecular crystals

Oral Lectures

09:30 - 09:50 **Kamil Tokár; Matej Uhliar; Mariana Derzsi** - *Advanced Technologies Research Institute, Faculty of Materials Science and Technology in Trnava, Slovak University of Technology in Bratislava; Institute of Physics, Slovak Academy of Sciences, Slovakia*
The first silver chloride with rare silver clusters from *ab initio* study

09:50 - 10:10 **Michal Novotný; František Karlický** - *Department of Physics, Faculty of Science, University of Ostrava, Czech Republic*
Chemistry of Mxene terminal groups and their effect on layer cohesion

10:10 - 10:30 Coffee break

Chair:

Invited Lecture

10:30 - 11:00 **Maren Podewitz** - *Institute of Materials Chemistry, TU Wien, Vienna, Austria*
Predicting Reactivity and Selectivity of Transition-Metal Catalysts - Improving Accuracy Beyond Electronic Structure Theory

Oral Lectures

11:00 - 11:20 **M. Biela, E. Klein** - *Department of Chemical Physics, Slovak University of Technology in Bratislava, Slovakia*
Mechanisms of antioxidant action of phenolic acids and their carboxylate anions

11:20 - 11:40 **Johannes Hoja; A. Daniel Boese** - *University of Graz, Austria*
Benchmarking anharmonic vibrational frequencies of molecular dimers

11:40 - 12:00 **Vladimir Malkin, Florian Lemken, Stanislav Komorovsky, Olga Malkin** - *Institute of Inorganic Chemistry, Slovak Academy of Sciences, Slovakia*
Visualization of EPR Hyperfine Structure Coupling Pathways

12:00 - 12:05 Closing

12:05 - Lunch

Poster section

7th September (Wednesday) P1 - P19
8th September (Thursday) P20 - P38

P1 **Ahmed Shaalan Alag; Dávid P. Jelenfi, Attila Tajti; Péter G. Szalay** - *György Hevesy Doctoral School, ELTE Eötvös Loránd University, Hungary*
Accurate evaluation of coupled cluster ionization potentials and electron affinities via excitation energy calculations

P2 **Nissrin Alharzali, Hisham Khalifeh Al Rawas, Sonia Taamalli, Abderrahman El Bakali, Florent Louis, Ivan Černušák, Duy Quang Dao** - *Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Slovakia*
A theoretical study of the OH-initiated atmospheric degradation of pentachlorophenol.

P3 **Andrej Hurajt, Martin Znava, Beatrice Karg, Mina Maddah, Magdalena Kowalska, Andrej Antusek** - *ATRI, Slovak University of Technology, Bratislava, Slovakia*
NMR shielding calculations of beta-NMR probe nuclei in ionic liquids.

P4 **Bónis Barcza; Ádám B. Szirmai; Attila Tajti; Péter G. Szalay** - *ELTE Eötvös Loránd University, Institute of Chemistry, Hungary*
Comparison of different model potentials for non-covalent interactions between N-heterocycles in ground and excited state

P5 **Johannes Hoja; Alexander List; A. Daniel Boese** - *Institute of Chemistry, University of Graz, Austria*
Development and Assessment of QM:QM Methods for Molecular Crystals

P6 **Martin Breza** - *Faculty of Chemical and Food Technology STU, Bratislava, Slovakia*
DFT studies of dimethyl amino phenyl substituted silver phthalocyanine

P7 **Šimon Budzák; Jakub Joniak; Henrieta Stankovičová; Milan Sýkora; Katarína Gaplovská-Kyselá; Marek Cigáň** - *Department of Chemistry, Matej Bel University, Banská Bystrica, Slovakia*
Rigidized 3-aminocoumarin fluorescent pH probes for acidic conditions

P8 **S. Forndran, N. Bersenkowitsch, C. van der Linde, M. Ončák, M. K. Beyer** - *Institut für Ionenphysik und Angewandte Physik, Leopold-Franzens-Universität, Innsbruck, Austria*
Photodissociation of sodium iodide clusters doped with 5-bromovalerate

P9 **Michael Hütter; Ethan Cunningham; Christian van der Linde; Martin K. Beyer; Milan Ončák** - *Institute for Ion- and Applied Physics, University of Innsbruck, Austria*
Photoinduced charge-transfer processes in cesium iodide cluster ions

P10 **Dominik Jank; Miriam Meyer; Arne Schiller; Paul Scheier; Andrew Ellis; Milan Ončák** - *Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria*
Vibrational and Electronic Spectroscopy of $(C_{60})_n^{\pm}$-Clusters.

P11 **Erik Kalla, Hugo Semrád, Miriama Mateášová and Markéta Munzarová** - *Department of Chemistry, Masaryk University*
DFT Analysis of Diels-Alder Reactions for the preparation of forskolin derivatives

P12 **Joseph Kfoury; Frank Blockhuys; Julianna Oláh** - *Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Hungary*
Understanding the Effect of the Transition Metal on the Properties of Cyclopentadienyl-stabilized 5,1,3,2,4-Metalladithiadiazoles

P13 **Ahmed M. Rozza; Mary Jo Ondrechen; Julianna Oláh** - *Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economic, Hungary*
Effect of dual phosphoprylation on the activation mechanism of ERK2: computational insights

P14 **Andrea Kováčová** - *Department of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Slovak Republic*
On quantum chemical calculations of acidity constant of phenol derivatives and their cation radical forms

P15 **Ádám Margócsy; Ágnes Szabados** - *ELTE Eötvös Loránd University, Faculty of Science, Institute of Chemistry, Hungary*
A novel treatment of redundancy in Multi-Configuration Perturbation Theory

P16 **Ján Matúška; Lukáš Bučinský, Marek Štekláč, Marián Gáll; Michal Pitoňák** - *Institute of Physical Chemistry and Chemical Physics FCFT SUT, Bratislava, Slovakia*
Prediction of docking scores to the main protease M^{pro} by machine learning

P17 **Adèle D. Laurent, Habiburrahman Zulfikri, Claudia Filippi, Miroslav Medveď** - *Department of Chemistry, Faculty of Natural Sciences, Matej bel University, Slovakia; RCPTM CATRIN, Palacky University Olomouc, Czech Republic*
Computational insights into photochromic behavior of iminothioindoxyls

P18 **Martyna A. Osada; Michał Tomza** - *University of Warsaw, Poland*
Accurate *ab initio* calculations for the alkali-metal and alkaline-earth-metal hydrides

P19 **Tomáš Ovad; Marin Sapunar; Štěpán Sršeň; Petr Slavíček; Zdeněk Mašín; Juraj Fedor** - *University of Chemistry and Technology, Prague, Czech Republic*
Excitation and fragmentation of SF_6-replacement dielectric gas C_3F_7CN: electrons vs. photons

P20 **Kemal Önen; Dennis F. Dinu; Klaus R. Liedl** - *Department of General, Inorganic and Theoretical Chemistry, University of Innsbruck, Austria*
Decomposition of normal coordinates and harmonic vibrational frequencies

P21 **Ondřej Demel; Jakub Višňák, Jakub Lang, Andrej Antalík, Jan Brandejs, Jiří Brabec, Libor Veis, Mihály Máté, Örs Legeza, Jiří Pittner** - *J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Czech Republic*
Multireference and relativistic DMRG-tailored CC methods.

P22 **Marin Sapunar; Petr Slavíček; Zdeněk Mašín** - *Department of Physical Chemistry, University of Chemistry and Technology; Institute of Theoretical Physics, Charles University, Prague, Czech Republic*
Born approximation in the context of electron energy loss spectroscopy

P23 **Jonas Schlagin; Dennis F. Dinu; Thomas Loerting; Klaus R. Liedl** - *Department of General, Inorganic and Theoretical Chemistry, University of Innsbruck, Austria*
Ab initio calculations of anharmonic vibrational spectra of carbonic acid and carbonic acid methyl ester

P24 **Jutta S. Schnizer, Magdalena Salzburger, Christian van der Linde, Martin K. Beyer, Milan Ončák** - *Institut für Ionenphysik und Angewandte Physik, Leopold-Franzens-Universität Innsbruck, Austria*
Structure and spectroscopic properties of hydrated O_2^- and O_3^- ions

P25 **Gabriel R. Schöpfer; Ethan M. Cunningham; Martin K. Beyer; Milan Ončák** - *Institut für Ionenphysik und Angewandte Physik, Leopold-Franzens-Universität Innsbruck, Austria*
Dissociation pathways of hydrated magnesium sulfate clusters $[Mg_n(SO_4)_{n-1}(H_2O)_m]^{2+}$

P26 **Renata Sechi; Tibor Höltz** - *Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economic; Furukawa Electric Institute of Technology, Nanomaterials Science Group, Hungary*
DFT study of CO_2 activation on $Pd_xPt_{(4-x)}$ clusters in the gas phase

P27 **Ján Šimunek; Jozef Noga** - *Department of Inorganic Chemistry, Faculty of Natural Sciences, Comenius University, Slovakia*
Running Hartree-Fock calculations in local molecular orbitals.

P28 **Karlo Sović; Ines Primožič; Tomica Hrenar** - *Department of Chemistry, University of Zagreb Faculty of Science, Croatia*
Conformational analysis of quinuclidin-3-one derivatives

P29 **Marek Štekláč; Lukáš Bučinský; Marián Gáll; Ján Matúška; Michal Pitoňák** - *Institute of Physical Chemistry and Chemical Physics FCHPT STU, Bratislava, Slovakia*
Potential inhibitors of SARS-CoV-2 proteases

P30 **Martin Šulka; Katarína Šulková; Matúš Dubecký** - *Advanced Technologies Research Institute, Faculty of Materials Science and Technology in Trnava Slovak University of Technology in Bratislava, Slovakia*
Assessing the accuracy of Quantum Monte Carlo in hydrogen-bonded and strongly correlated systems.

P31 **Katarína Šulková; Martin Šulka; Andrej Antušek** - *Advanced Technologies Research Institute, Faculty of Materials Science and Technology in Trnava Slovak University of Technology in Bratislava, Slovakia*
Exploring water adsorption and reactivity in a series of doped aluminum cluster anions

P32 **Ádám B. Szirmai; Bónis Barcza; Attila Tajti; Péter G. Szalay** - *ELTE, Eötvös Loránd Uninversity, Institute of Chemistry, Hungary*
Theoretical description of interacting chromophores

P33 **Nina Tokić, Tomislav Piteša, Marin Sapunar, Nađa Došlić** - *Faculty of Science, Department of Physics, Croatia*
What can we learn by comparing surface hopping algorithms?

P34 **Barbora Vénosová; František Karlický** - *Department of Physics, Faculty of Science, University of Ostrava, Czech Republic*
MXene quantum dots: Effect of surface/edge functionalization on their optical properties

P35 **D. Vrška, P. Neogrády, V. Kellö, M. Urban, M. Pitoňák** - *Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University, Slovakia*
Excited states of auro-carbons: CASPT2 and CCSD(T) calculations of C_2Au_2 and C_2Au_4

P36 **Maks Walewski; Matthew D. Frye; Michał Tomza** - *Faculty of Physics, University of Warsaw, Poland*
Quantum interference effects in cold Rb–Sr^+ collisions high above the ultracold regime

P37 **Aleksander P. Woźniak; Maciej Lewenstein; Robert Moszyński** - *Faculty of Chemistry, University of Warsaw, Poland*
Effects of electronic correlation on the high harmonic generation in helium

P38 **Bárbara Zamora; László Nyulászi; Tibor Höltzl** - *Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Hungary*
DFT-based investigation of structure and CO_2 adsorption on zinc dopped copper clusters