List of posters of the poster session A

(first 73 posters are part of the poster competition presented by PhD students)

PA1 **Aguirre, T. N.**: *Fast estimation of superconducting critical temperature of hydrogen-based binary and ternary systems*

PA2 **Allgöwer, F.**: *How Light-Driven Redox Reactions Modulate Proton Transfer Barriers in Photosystem II*

PA3 **Andersen, J.**: *Circular dichroism through the lens of coupled-cluster methods*

PA4 **Audinet, T.**: *One dimensional model for relativistic quantum chemistry*

PA5 **Bao, S.**: *Time-dependent Vibrational Electronic Coupled Cluster (VECC) theory for non-adiabatic dynamics*

PA6 **Barcza, B.**: *New investigation of ab initio fragment models to study the excited states of interacting chromophores*

PA7 **Bauer, M.**: *Excitonic Renormalization towards Modular Large-scale ab initio Electronic-structure Calculations*

PA8 **Baumgarten, M.**: *Nonorthogonal and Overcomplete Hilbert Spaces for Quantum Monte Carlo Methods*

PA9 **Belina, M.**: *Proton Transfer in the Pyrrole-Water System: Relaxation after Double Ionization*

PA10 **Berrade, A. E. I.**: *Multi-Resonant TADF via N and B doped Triangulenes*

PA11 **Bharadwaz, P.**: *Reactivity factors in catalytic methanogenesis and their tuning upon coenzyme F430 biosynthesis*

PA12 **Bonometti, L.**: *Diffusion Coefficient of Lithium in Cathode Materials for Lithium Ion Batteries from DFT, Metadynamics and Post-HF*

PA13 **Bovolenta, G.**: *Comprehensive Quantum Chemistry Approach for the Evaluation of Binding Energies on Interstellar Ices. From the Water Dimer to Far-Reaching Surfaces.*

PA14 **Briganti, V.**: *Uncertainty aware active learning for linear machine learning force fields*

PA15 **Burgess, A.**: *A DFT+U-type functional to correct both self interaction error and static correlation error*

PA16 **Carroll, L.**: *Self-organization, Restructuring and Reactivity: Computational Modelling of Catalysis on Nanoporous Gold using AIMD Simulations*

PA17 **Cebreiro, A.**: *Calculation of the g-tensor with the RAS-CI method*

PA18 **Chakraborty, R.**: *Embedding Pair Coupled Cluster Doubles–Based Methods in DFT*

PA19 **Chaussy, L.**: *Spectroscopy of Copper-Superoxo Complexes: a Revival Based on Correlated Methods*

PA20 **Chen, Y.**: *Multi-configurational nature of electron correlation within nitrogen vacancy centers in diamond*

PA21 **Chirchir, G.**: *Electronic and Mechanical Properties of Re Doped* $FeMnP_{0.67}A_{0.33}$ *(A=Ga and Ge)*

PA22 **Chuiko, V.**: *A Size-Consistent Wavefunction Ansatz Built from Statistical Analysis of Orbital Occupations*

PA23 **Cieśliński, D.**: *First-order symmetry-adapted perturbation theory for electronically degenerate states*

PA24 **Cigrang, L.**: *Modelling photodissociation using non-adiabatic, on-the-fly quantum dynamics simulations*

PA25 **Comas i Vilà, G.**: *Does Serial Femtosecond Crystallography Depict State-Specific Catalytic Intermediates of the Oxygen-Evolving Complex?*

PA26 **Craciunescu, L.**: *Theoretical investigation of bimolecular collisions:* $NO + CO_2$

PA27 **Crisci, L.**: *Toward a black-box computation of accurate rate constants for barrierless processes: new hints for a challenging problem*

PA28 **Csizi, K.-S.**: *Interactive quantum magnifying glass with quantum-classical hybrid models*

PA29 **Csoka, J.**: *Analytic gradients for local density fitting Hartree–Fock and Kohn–Sham methods*

PA30 **Cunha, R. D.**: *Multiscale investigation of the structural basis for photoacclimation in the cryptophyte alga PC577 and PE545 antenna complexes*

PA31 **Danilov, D.**: *Spin-orbit coupling in an Ehrenfest non-adiabatic dynamics framework*

PA32 **Deng, S.**: *Device simulation of high performance wet power for sunlight coordination under natural conditions*

PA33 **de Lima, L. W.**: *Copolymerization of Carbon Dioxide and Cyclohexene Oxide by Bimetallic Homogeneous Catalysts: A DFT Study of its Reaction Mechanism*

PA34 **Diaz, G. S.**: *How well do alternative formulations of Rowe's equation of motion perform for atomic and molecular transition energies?*

PA35 **Didovets, Y.**: *Shape memory polymers – the role of hydrogen bonds: ab initio molecular dynamics simulations and energy decomposition analysis*

PA36 **Ditte, M.**: *Non-covalent interactions obtained from quantum embedding of electronic system in charged quantum harmonic oscillators*

PA37 **Di Grande, S.**: *The parameter-free junChS-F12 model: a cost-effective approach for accurate calculations of structural, spectroscopic and thermochemical molecular properties*

PA38 **Dominguez, J.**: *An unexpected problem of astrochemical significance and a healing strategy*

PA39 **Drontschenko, V.**: *Analytical Second Order Properties for the Random Phase Approximation: Accurate and Efficient Computation of Nuclear Magnetic Resonance Chemical Shieldings*

PA40 **Dua, P.**: *Mechanism for CO_2 cycloaddition reaction using a tetranuclear 3d-4f helicates as an efficient catalyst: A DFT and ab-initio exploration*

PA41 **Eduardus, E.**: *Towards Detection of The Molecular Parity Violation in Helical Ferrocene, Ruthenocene, and Osmocene*

PA42 **Eeckhoudt, J.**: *Conceptual Density Functional Theory under Isotropic Pressure: Towards Diatomic Molecules*

PA43 **Ergün, Ö.**: *Förster Resonance Energy Transfer Applied to Drug Design*

PA44 **Fatkova, K.**: *Towards the Singlet Fission Quantum Yield*

PA45 **Fauser, S.**: *Chemical Accuracy at Low Computational Cost with σ-Functionals for the Kohn-Sham Correlation Energy*

PA46 **Feldmann, R.**: *Nuclear-Electronic Hartree-Fock Density Matrix Renormalization Group*

PA47 **Filgas, J.**: *Nuclear Quantum Effects in Photochemical Reactivity*

PA48 **Fitzpatrick, A.**: *Orbital Optimised Variational Quantum Eigensolver*

PA49 **Fu, W.**: *Towards the ground state of molecules via diffusion Monte Carlo on neural networks*

PA50 **Gastearena, X.**: *Computational study of the Lewis acid-catalyzed zwitterionic ring-expansion polymerization (ZREP) of monosubstituted epoxides*

PA51 **Ge, Y.**: *Computational Method for Evaluating the Thermoelectric Power Factor for Organic Materials Modeled by Holstein Model: A Time-Dependent Density Matrix Renormalization Group Formalism*

PA52 **Gerasimov, I.**: *A broad class of semi-local DFT ingredients from fractional calculus*

PA53 **Gešvandtnerová, M.**: *Heterogeneous catalysis by acidic zeolites: DFT study of isobutanol to butenes transformations*

PA54 **Giudetti, G.**: *AIMD-based protocol for modeling exciplex fluorescence spectra: OPPn example*

PA55 **Glaser, N.**: *A DMRG-based framework for large-scale anharmonic vibrational calculations*

PA56 **Goger, S.**: *Exploring the Interaction of Molecular Dipole Polarizability and Frontier Orbital Energies in Chemical Compound Space*

PA57 **González, J. R.**: *Effect of the bridge between the two rings in biphenil-like systems in the dyson orbitals*

PA58 **Gorges, J.**: *Quantum chemical calculation of mass spectra via automated transition state search*

PA59 **Grazioli, L.**: *From Magnetic Circular Dichroism to Magnetic White Dwarfs: challenges in the calculation of properties in a magnetic field, using Coupled-Cluster and Unitary Coupled-Cluster Theory*

PA60 **Greiner, J.**: *Exploiting Point Group Symmetry, Screening and Error Estimation in Many-Body Expanded Full Configuration Interaction*

PA61 **Gutierrez-Cañas, M. L.**: *Solvent effects of choline and geranate-based ionic liquid on organic catalysts*

PA62 **Győri, T.**: *Automated development of PESs via active learning: a real-world stress test of electronic structure theories and implementations?*

PA63 **Haberhauer, J.**: *Investigation of a PLATICT system as potential molecular motor*

PA64 **Halder, D.**: *Development of a compact ansatz for near term quantum algorithms*

PA65 **Hasecke, L.**: *Deeper into the quantum realm*

PA66 **Hennefarth, M.**: *Linearized Pair-Density Functional Theory*

PA67 **Herok, C.**: *Describing (Di-)Anionic Species in Solution: A Benchmark Study*

PA68 **Hillers-Bendtsen, A. E.**: *Probing the Ultrafast Photodynamics of Dihydroazulene with In Silico Time Resolved Photoelectron Spectroscopy and Ultrafast Electron Diffraction*

PA69 **Hlavacova, R.**: *Prediction of solid-state properties of superheavy elements*

PA70 **Hlinčík, A.**: *Theoretical study of Cr-Cr bonding interactions, the SIYNAQ case study*

PA71 **Hou, X.**: *Epistatic Variations in the Omicron Receptor Binding Domain Can Enhance Host Recognition: An In Silico Assessment and Prediction*

PA72 **Hou, Y.**: *Development of Machine Learning Potentials and Implementations of Molecular Dynamics and Infrared Spectra Simulations in MLatom*

PA73 **Jaďuďová, D.**: *Photophysical properties of molecular fluorophores in carbon dots*

PA74 **Aazaad, B.**: *Interstellar reaction mechanisms of Glycolaldehyde*

PA75 **Abraham, V.**: *Estimating the accuracy of pseudopotential based GW method at different levels of self consistency using Gaussian orbitals*

PA76 **Abulyaissova, L.**: *A Quantum Chemical Insight into Adsorption Interaction of PVA with Copper Oxide*

PA77 **Ahmadkhani, S.**: *The Linear Response Pair Coupled Cluster Doubles Theory*

PA78 **Aidas, K.**: *Structural and NMR Properties of Ionic Liquid Systems Modelled by an Integrated MD-QM/MM Approach*

PA79 **Alessio, M.**: *Quantum Chemical Study of Nickelocene: From Magnetic Molecules to Materials*

PA80 **Alharzali, N.**: *Theoretical study of OH-initiated decomposition of chlorpyrifos in the gaseous and aqueous phases*

PA81 **Andrae, D.**: *Properties of Isolated Small Molecules, Molecular Ions and Molecular Clusters – Theory vs. Experiment*

PA82 **Angappan, M. P.**: *Atmospheric degradation of the oxidation products of monoterpenes emitted by plants*

PA83 **Aniban, X.**: *A New Perspective on Dispersion Interaction Density: o-DID*

PA84 **Antalik, A.**: *Unleashing MiMiC: Making the scalable and flexible QM/MM framework truly versatile*

PA85 **Asher, J.**: *Photoisomerisation and Relaxation of Variously-Substituted Quinazolinone-based Schiff Bases*

PA86 **Bader, F.**: *Taylor expansion-based polyspherical kinetic energy operators in vibrationally correlated calculations*

PA87 **Bajaj, A.**: *Metal-Ligand Covalency Trends in Actinide Complexes*

PA88 **Bende, A.**: *Intermolecular-type conical intersections in benzene and catechol dimers*

PA89 **Bensberg, M.**: *Corresponding Active Orbital Spaces along Chemical Reaction Paths*

PA90 **Beran, G.**: *Designing Organic Photomechanical Engines with Exceptional Work Capacities Through Quantum Chemistry*

PA91 **Berraud-Pache, R.**: *Modelling the interaction of a natural red dye with wool during the dyeing process*

PA92 **Biczysko, M.**: *The Q|R Project: Quantum-Based Refinement of Biomacromolecules*

PA93 **Avila-Blanco, G.**: *The 12D vibrational states of CH_4Ar and CH_4F^- computed with a 9D contracted intramolecular basis set*

PA94 **Bleken, F. L.**: *Understanding $Si(CH_3)_2Cl_2$ formation on a Cu rich model surface in the Rochow-Müller process*

PA95 **Boese, A. D.**: *QM:QM Methods for Molecular Crystals*

PA96 **Bokarev, S.**: *Electron dynamics and (auto)ionization in highly-excited molecules*

PA97 **Boto, R. A.**: *Addressing the effect of the chemical structure on the coherence times of electron spin qubits in graphene nanofragments*

PA98 **Bourne-Worster, S.**: *Quantum Dynamics of Excited State Proton Transfer in Green Fluorescent Protein*

PA99 **Branzanic, A.**: *Why does sulfite reductase employ siroheme?*

PA100 **Breza, M.**: *DFT studies of the cytotoxicity of the anticancer drug SN-38*

PA101 **Brothers, E.**: *Underappreciated Errors in DFT Reaction Barriers*

PA102 **Bucinsky, L.**: *Relativistic Quantum Crystallography of Hg atom and Hg compounds withX-ray Constrained Wavefuncion fitting*

PA103 **Budzák, Š.**: *Thermal isomerization of phenylazoindoles: Inversion or rotation?*

PA104 **Cao, C.-S.**: *Ab initio Quantum Simulation of Strongly Correlated Materials with Quantum Embedding*

PA105 **Cardenas, C.**: *Electron Localization (Function) in the Excited State with Single Determinant Methods*

PA106 **Casanova, D.**: *Anti-Kasha Emission Triggered by J-Coupling and Molecular Rigidity*

PA107 **Cernusak, I.**: *How do behave catenanes built from cyclo[18]carbon rings under tension?*

PA108 **Chai, Z.**: *Grand canonical ensemble approaches for modeling electrochemistry in CP2K*

PA109 **Chen, X.**: *Theoretical models of electron transfer and energy transfer in photocatalysis*

PA110 **Chen, Z.**: *Electron transfer theory based on diabatic representation*

PA111 **Cunha, A.**: *Structure and Dynamics of a VHL-recruiting PROTAC*

PA112 **Delcey, M.**: *Variational optimization of multiconfigurational pair-density functional theory*

PA113 **Jassar, M. B.**: *Benchmarking Semi-Empirical Methods for the Li-Ion battery Solid Electrolyte Interphase*

PA114 **de Busturia, D. C.**: *Polarizable Embedding Potentials Through Molecular Fractionation with Conjugate Caps Including Hydrogen Bonds*

PA115 **De Chavez, D.**: *Inner Projection-based Integral Evaluations using One-Centered Corrected Two-Electron Integrals*

PA116 **de Haas, T.**: *Surface Hopping Dynamics of Excited-State Proton-Coupled Electron Transfer*

PA117 **de Moura, C. E. V.**: *An Efficient Spin-Free Formulation of the Multireference Algebraic Diagrammatic Construction Theory for Core Excited States*

PA118 **De Santis, M.**: *Environmental Effects via Multilevel Embedding Approaches in the Real-Time Time-Dependent Density Functional Theory*

PA119 **de Souza, B.**: *On the importance of conformational Entropy when predicting Chemistry: results from the new Global Optimizer AlgoriThm (GOAT) implemented in ORCA*

PA120 **Ding, L.**: *Information-Assisted Complete Active Space Optimization (i-CAS)*

PA121 **Doslic, N.**: *Light Induced Processes in Uracil and Uracil Dimer Stacks in the Gas Phase and in Solution*

PA122 **do Casal, M. T.**: *Anti-Kasha Photochemistry in Indigo Carmine*

PA123 **East, A.**: *Predicting ligand-exchange free energies in solution: The chelate effect*

PA124 **Eckhoff, M.**: *Lifelong Machine Learning Potentials*

PA125 **Ehlert, C.**: *Metal-Free Molecular Catalysts for the Oxygen Reduction Reaction: Electron Affinity as an Activity Descriptor*

PA126 **Eng, J.**: *Joint Experimental and Theoretical Inverstigation of Excited State Vibrational Coherences in Mn Single Molecule Magnets*

PA127 **Erhard, J.**: *Kohn-Sham Inversion Using Techniques from the Optimized Effective Potential Method .*

PA128 **Fantuzzi, F.**: *Electronic Structure, Bonding and Reactivity of Emerging Boron-Based Systems: Insights from Theory*

PA129 **Ferenc, D.**: *Pre-Born–Oppenheimer Dirac–Coulomb–Breit computations for two-fermion systems*

PA130 **Filip, M.-A.**: *Developing Hybrid Quantum Monte Carlo Algorithms for Low Quantum Overheads and Improved Noise Resilience*

PA131 **Floris, F. M.**: *On the solvatochromic effect due to Pauli repulsion and dispersion solute–solvent interaction*

PA132 **Foerster, A.**: *Large scale GW-BSE calculations with explicit treatment of spin-orbit effects*

PA133 **Djumayska, S.**: *TD-DFT modeling of TADF blue light emitters*

List of posters of the poster session B

(first 73 posters are part of the poster competition presented by PhD students)

PB1 **Hunter, G.**: *Monte Carlo Simulations of Copper using Machine Learning Potentials*

PB2 **Hurajt, A.**: *Advancing β-NMR Spectroscopy: Computational Modeling of NMR Shielding of Ions in Ionic Liquids*

PB3 **Højlund, M.**: *Adaptive basis sets for time-dependent bivariational wave functions: Linear, polar and exponential parametrization of single-particle functions*

PB4 **Høyer, N. M.**: *Quantum molecular dynamics with a time-dependent adaptive density-guided approach for potential energy surface construction*

PB5 **Illobre, P. G.**: *Fully Atomistic Model to Compute Fluorescence Enhancements Near Plasmonic Materials*

PB6 **Jahani, S.**: *New insight into polyanilines' electronic structures and properties augmented with orbital correlations*

PB7 **Jaroš, A.**: *Actinide-actinide bonding in fullerenes: A DFT nightmare*

PB8 **Javaheri Moghadam, M.**: *Measuring local correlations in biomolecular systems using quantum information theory*

PB9 **Jayadev, N. K.**: *The regular and resonant Auger spectrum of benzene*

PB10 **Jaykhedkar, N.**: *Assessing the effects of dispersion corrections on the temperature dependent structural properties of $SrZrS_3$ phases*

PB11 **Jensen, A. B.**: *Efficient time-dependent vibrational coupled cluster computations with time dependent basis sets at the two-mode coupling level*

PB12 **Jensen, R. B.**: *Runtime for Vibrational Structure on Quantum Computers*

PB13 **Jiang, T.**: *Matrix Product State Algorithms for Response Function of Quantum Many-body Systems*

PB14 **Jiménez, J. A. R.**: *Dynamic correlation into CASSCF wave functions by means of an effective potential.*

PB15 **Jingar, R.**: *Efficient and accurate relativistic ab initio calculations of electric and magnetic dipole transitions in Eu3+ complexes*

PB16 **Joshi, P.**: *Generalized perturbative orbital relaxation correction based on random phase approximation*

PB17 **Jíra, T.**: *Representative Sampling of Time-Resolved Electronic Spectra for Stilbene*

PB18 **Jørgensen, F. K.**: *Singlet linear response for open-shell transition metals – extending the multiconfigurational short-range density functional theory*

PB19 **Kaczun, T.**: *Enabling OF-DFT with Machine Learning? A novel ansatz for data generation*

PB20 **Kalvoda, T.**: *Exploring the conformational space of short peptides: A way to understand protein folding?*

PB21 **Khanifaev, J.**: *The effect of machine learning predicted anharmonic properties in Quantum Cluster Equilibrium calculations*

PB22 **Kircher, J.**: *Benchmarking under uncertainty - Towards the prediction of polar organic reactivity*

PB23 **Kitzmiller, N.**: *Extending the Concordant Mode Approach (CMA)*

PB24 **Kjeldal, F.**: *Decomposing Chemical Space: Applications for Machine Learning*

PB25 **Kneiding, H.**: *Evolutionary Multiobjective Optimization for Transition Metal Complexes*

PB26 **Knysh, I.**: *BSE formalism vs TD-DFT: Dipole moments of increasingly long push-pull oligomers*

PB27 **Kohn, J.**: *Efficient Calculation of Coupling Integrals with the Dimer Projection Method (DIPRO) using density-matrix (P) tight-binding (TB)*

PB28 **Komando, L.**: *Redox potentials of iron III oxides in presence of ionic liquids and citrate anions. Quantum-chemical studies.*

PB29 **Kováčová, A.**: *Quantum chemical evaluation of electrochemical oxidation potentials of phenol derivatives: Chemical accuracy of implicit SMD solvent model*

PB30 **Kumar, P.**: *Modeling phosphorescent properties of Heteroleptic Ir (III) complexes with Local coupled-cluster method and DFT*

PB31 **Kumar, R.**: *A Computational Framework for Designing Molecular Electronic Breadboards*

PB32 **Kumar, V.**: *On the convergence behaviour of different Optimised Effective Potential methods*

PB33 **Kvedaraviciute, S.**: *Enabling fully polarizable multiscale QM/MM simulations through MiMiC*

PB34 **Lafiosca, P.**: *Fully polarizable Molecular Mechanics/Frozen Density Embedding approach for magnetic properties*

PB35 **Le, V.**: *PyOpenRSP: Analytic Molecular Response Properties for Spectroscopy*

PB36 **Leadbeater, C.**: *Non-unitary Trotter circuits for imaginary time evolution*

PB37 **Lee, N.**: *Strongly correlated states have a simple structure*

PB38 **Leitner, J.**: *The fourth-order algebraic diagrammatic construction scheme for the polarization propagator*

PB39 **Lemke, Y.**: *Ascending Jacob's Ladder of Beyond-RPA Methods with Highly Accurate σ- and τ-Functionals with Approximate Exchange Kernels*

PB40 **Lemken, F.**: *Combined Hückel and Perturbation Theory Approach for the Prediction of π Contributions to Indirect Spin-Spin Coupling in Conjugated Hydrocarbons*

PB41 **Liebert, J.**: *N-representability problem for excited states*

PB42 **Ligorio, R. F.**: *GruPol: estimating electrostatic and electro-optic properties of macromolecules*

PB43 **Lindic, T.**: *Fluorination of Small Carbon Based Molecules on a NiF_2 Model Surface: a First-Principles and AIMD Approach*

PB44 **Lodeiro, L. N.**: *Mechanistic Insights into the DABCO-catalyzed Cloke-Wilson Rearragement: A DFT Perspective*

PB45 **Loja, A. D. M.**: *Computational study on the photochemical stability of hydrogen bonds within acid dimers*

PB46 **Losada, I. B.**: *Intramolecular photoactivity and bimolecular electron transfer processes involving transition metal complexes revealed by DFT calculations*

PB47 **Loukili, M.**: *The effect of pressure on the [2+2] cycloadditions of ethylene*

PB48 **Luts, H.-E.**: *Halogen and chalcogen polyhydrides*

PB49 **Lévárdi, Á.**: *Automated modeling of reaction networks of bullvalene*

PB50 **Maisuradze, T.**: *From Rare to Earth-Abundant Transition Metal Photoactive Complexes: Long-lived Excited States of CoCCs*

PB51 **Martinka, J.**: *Photodissociation of vinylbromide: a non-adiabatic molecular dynamics and machine learning study*

PB52 **Mattos, R. S.**: *Quantum dynamics from Classical Trajectories*

PB53 **Matz, F.**: *Molecular Auger Decay Rates from Complex-Variable Electronic-Structure Methods*

PB54 **Mena, Y. A. C.**: *Electronic molecular parameters for new-physics searches in the $BaCH_3$ and $YbCH_3$ symmetric top molecules*

PB55 **Merritt, I.**: *Nonadiabatic Coupling in Trajectory Surface Hopping: How Approximations Impact Excited-State Reaction Dynamics*

PB56 **Meyr, J.**: *Unraveling the Mechanism of Covalent Lysine Attachment to Wortmannin: Insights from QM/MM studies*

PB57 **Miron, G. D.**: *CO lock mechanism can explain the presence of Fluorescence in Non Aromatic Systems*

PB58 **Moerman, E.**: *Reaching the thermodynamic limit of band gaps in the equation-of-motion coupled-cluster framework*

PB59 **Monzel, L.**: *The path from rotations to vibrations. The quantum rotor in a magnetic field.*

PB60 **Morgan, D.**: *Scalable and efficient ab initio X-ray spectroscopy calculations with numeric atomic orbitals*

PB61 **Motoki, K.**: *Beyond Born-Oppenheimer pharmaceutical quantum chemistry of thalidomide analogs and deuterium substituents*

PB62 **Mráziková, K.**: *QM investigation of phosphine synthesis in Venus' atmosphere*

PB63 **Mueller, M.**: *An efficient and non-iterative method for large-scale screening applications combining DFT and semiempirical quantum mechanics*

PB64 **Mörchen, M.**: *Autonomous Active Space Calculations through AutoCAS*

PB65 **Müllerová, S.**: *Interaction of iron and chromium decorated circumcoronenes with hydrogen molecules – dissociation and side on/end on binding modes*

PB66 **Nadoveza, N.**: *Analytical Canonic Polyadic representation of the potential energy surface for reactive scattering of CH_4 on Ni(111) (13D)*

PB67 **Narayanan S J, J.**: *Shape Resonances of Uracil: The Effect of Microhydration*

PB68 **Nemirovich, T.**: *Bridging Electrochemistry and Photoelectron Spectroscopy in the Context of Birch Reduction*

PB69 **Netz, J.**: *Electronic structure of a radical bridged dinuclear cobalt(II) single-molecule magnet*

PB70 **Nguyen, V. H. A.**: *High-throughput exploration of the chemical space for single molecule magnets discovery*

PB71 **Nowak, D.**: *The application of machine learning methods to the prediction of novel ligands for RORγ/RORγT receptors*

PB72 **Oliveira, L.**: *Photochemistry and Proton Transfer Mechanisms in 2,6-Diamino-8-Azapurine*

PB73 **Polena, J.**: *Electron-induced chemistry: The case of azobenzene*

PB74 **Hall, M.**: *Noncovalent Control in Transition Metal Reactions*

PB75 **Jordan, K.**: *Strategies for Accurate Calculation of Positron Binding Energies of Positron-Atom and Positron-Molecule Complexes*

PB76 **Li, S.**: *Advances in Electronic Structure Methods*

PB77 **Liu, W.**: *The SDS Family of Methods for Strongly Correlated Electrons*

PB78 **Michl, J.**: *Metalloporphenes, Antiaromatic Analogs of Graphene*

PB79 **Nakatsuji, H.**: *Quantum chemistry with accurate solutions of the Schrödinger equation*

PB80 **Fu, M.**: *How one-photon properties affect the entangled two-photon absorption*

PB81 **Gall, M.**: *Improved docking score predictions with a fragment-oriented multi-scale graph attention model*

PB82 **Ganguly, G.**: *UV-vis Spectra Simulation of Transition Metal Porphyrins using ab initio Multireference Wavefunction Methods*

PB83 **Gil, E. S.**: *Investigating the trans-azobenzene photodynamics with coupled-trajectories*

PB84 **Goletto, L.**: *Multilevel-based Coupled Cluster in Density Functional Theory*

PB85 **Gowland, D.**: *Ion-trap quantum computations of CF_4^+ fragmentation using InQuanto*

PB86 **Grabarz, A.**: *The Computational Insight into Fused Heterocycle-Based Triarylhydrazone Photoswitching Mechanism*

PB87 **Graf, D.**: *A Simple and Efficient Route towards Improved Energetics within the Framework of Density-Corrected Density Functional Theory*

PB88 **Granatier, J.**: *The extrapolation Atomic Natural Orbitals of basis set to complete basis set (CBS) limit*

PB89 **Guo, Y.**: *Multiconfigurational self-consistent field theory for large active space and spin-orbit coupling*

PB90 **Guo, Z.**: *Efficient quantum imaginary time evolution by drifting real time evolution: an approach with low gate and measurement complexity*

PB91 **Hapka, M.**: *Multiconfigurational symmetry-adapted perturbation theory combined with reduced density matrix functional theory*

PB92 **Harsha, G.**: *Effect of quasi-particle and full self-consistency on the GW method*

PB93 **He, J.**: *Ab initio study of laser driven ultrafast spin dynamics at 2D limit*

PB94 **Hofierka, J.**: *Many-body theory of positron interactions with polyatomic molecules*

PB95 **Hori, Y.**: *Characterization of the electronic and geometrical structures and the formation pathway in oxidized [NiFe]-hydrogenase*

PB96 **Huang, Z.**: *Orbital Expansion Variational Quantum Eigensolver: Efficient Simulation of Molecules with Shallow Quantum Circuit*

PB97 **Ivanova, A.**: *Influence of the long-range exchange in density functionals for the description of excited states of organic TADF blue emitters*

PB98 **Jankowska, J.**: *Two-photon nonadiabatic molecular dynamics: the second excitation impact on the cyclohexadiene photo-cycloreversion mechanism*

PB99 **Jelemenska, I.**: *Cobalt complexes of tetra dentate semicarbazones - A-DFT study*

PB100 **Jeszenszki, P.**: *Variational Dirac–Coulomb approach with explicitly correlated basis functions*

PB101 **Johnson, P.**: *Strong Electronic Correlation with Richardson-Gaudin States*

PB102 **Kadek, M.**: *Classical and quantum embedding theories for quantum chemistry on quantum computers: towards applications in life sciences*

PB103 **Kelterer, A.-M.**: *Photodissociation versus Brook Rearrangement in Acylsilanes*

PB104 **Khire, S.**: *Facilitating economic MP2-level gradient evaluation for large molecular clusters: An art of possible*

PB105 **Kiriakidi, S.**: *Three cycles in the $[MoO_2]^{2+}$-catalyzed reduction of nitroaromatics to anilines with pinacol. A computational study towards the valorization of biomass subproducts.*

PB106 **Kitsaras, M. P.**: *Atoms and Molecules in the atmospheres of magnetic White Dwarfs*

PB107 **Komorovsky, S.**: *Modern DFT methods for prediction of the EPR g-tensor and hyperfine coupling tensor of species containing heavy elements*

PB108 **Konecny, L.**: *Relativistic Quantum-Electrodynamical Density Functional Theory for Cavity Engineering of Excited States*

PB109 **Larsson, E.**: *A new quantum-based embedding model for one- and two-photon absorption*

PB110 **Liu, L.**: *Investigations of imine-based unidirectional light-driven molecular motors by using ab initio multiple spawning dynamics*

PB111 **Li Manni, G.**: *Quantum Anamorphosis: Unraveling Magnetic Interactions in Polynuclear Transition Metal Clusters*

PB112 **Lukeš, V.**: *Effect of Fluorination on Chemical and Electronic Structure of Selected Aromatic Molecules: DFT Study*

PB113 **Malcek, M.**: *Impact of heteroatom doping on the hydrogen binding performance of circumcoronenes*

PB114 **Malis, M.**: *Nonadiabatic processes in condensed phase systems with ΔSCF*

PB115 **Malkin, O.**: *Distinguishing "Through-Space" from "Through-Bonds" Contribution in Indirect Nuclear Spin-Spin Coupling*

PB116 **Malkin, V.**: *Transmission of spin-polarization by π-orbitals*

PB117 **Manna, D.**: *The Impact of the Solvent Dielectric Constant on Dative Bonded Systems*

PB118 **Margócsy, Á.**: *Towards a fully relativistic calculation of the Bethe logarithm for two-fermion systems*

PB119 **Mariano, A. L.**: *Numerical Calculation of Vibronic Coupling and Spin Relaxation in Open-Shell Coordination Compounds with Multi-Reference Wave-function Methods*

PB120 **Matito, E.**: *How Reliable Are Modern Density Functional Approximations to Simulate Vibrational Spectroscopies?*

PB121 **Matúška, J.**: *Influence of the molecular representation on prediction of docking scores and screening properties of the neural network*

PB122 **Medved, M.**: *Photoluminescence Centers in Carbon Nanodots Talk to Each Other*

PB123 **Michalík, M.**: *O–C bond dissociation enthalpies of methoxy group in substituted anisoles*

PB124 **Mihálka, É. Z.**: *Convergence improvement in the coupled-cluster framework — an alternative approach based on amplitude functions*

PB125 **Mondal, S.**: *Spin-phonon decoherence in solid state paramagnetic defects from first principles*

PB126 **Mori, H.**: *Machine Learning-Boosted Quantum Chemical Design of Ionic Liquids for CO_2 Absorption and Experimental Verification*

PB127 **Nagy, P.**: *Accurate and efficient CCSD(T)/CBS up to 1000 atoms: optimization of the local natural orbital approach and large-scale applications*

PB128 **Nandi, A.**: *Δ-Machine Learning Approach to Improve a DFT-Based PES to CCSD(T) Accuracy*

PB129 **Nava, P.**: *Ab-initio acccurate singlet-triplet energy differences of cobalt complexes*

PB130 **Orimo, Y.**: *First-principles simulations of multielectron dynamics under strong laser pulses on quantum computers*

PB131 **Parasuk, V.**: *Mechanism of CO_2 Conversion Catalyzed by Nickle-Complex Electrocatalysts*

PB132 **Parasuk, W.**: *Mechanism of Catalyzed CO_2 to Methanol Conversion by Ru-PNP Complex Assisted by Ethylenediamine*

PB133 **Walewski, M.**: *Quantum resonant effects in cold Rb–Sr^+ collisions high above the ultracold regime*

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PC2 **Bashir, S.**: *A DFT-D3 study of interactions of saponite and hectorite clay minerals with poly(2-methyl-2-oxazoline) (PMeOX) polymer*

PC3 **De Vriendt, X.**: *Capturing correlation in the spin frustrated H_3-ring using the generator coordinate method and spin-constrained generalized Hartree-Fock states*

PC4 **Habrovsky, R.**: *A new expansion of the Coulomb potential and linear r_{ij} terms*

PC5 **Janoš, J.**: *On the wavelength-dependent photochemistry of the atmospheric molecule CF_3COCl: Ground-state versus excited-state dynamics*

PC6 **Oswald, J.**: *Towards analytic coupled-cluster gradients for molecules in strong magnetic fields*

PC7 **Otukile, K.**: *A Comprehensive Theoretical Investigation of Selected Low-Temperature Hydrocarbon Combustion Reactions*

PC8 **Ozaydin, B.**: *On the impact of thermal fluctuations on the exciton structure of the PC612 and PC645 antenna complexes: A dual classical/quantum molecular dynamics simulations study*

PC9 **Palao, D. G.**: *Environment effects change FRET distributions in a fluorophore-tagged disordered protein*

PC10 **Panchagnula, K.**: *Exploring the parameter space of an endohedral atom in a cylindrical cavity*

PC11 **Papapostolou, A.**: *responsefun: A Python Package for Computing Arbitrary Response Properties in the Algebraic Diagrammatic Construction Framework*

PC12 **Patra, C.**: *Dimensionality Reduction in Electronic Structure Theory via Nonlinear Dynamics, Synergetics and Machine Learning: Classical and Quantum Computing Aspects*

PC13 **Paul, R.**: *In Silico Studies of Spin crossover systems on surfaces*

PC14 **Petry, S.**: *Modeling of blue light pathways in light harvesting complexes*

PC15 **Pinel, S. S.**: *Electronic Resonances in N_2^-*

PC16 **Piras, A.**: *Predicting adsorbent and electronic properties of nanographenes*

PC17 **Pérez, A. F.**: *Computation of Auger decay widths with complex-variable coupled-cluster theory: benzene and zinc as case studies.*

PC18 **Pöverlein, M.**: *QM/MM Free Energy Calculations of Long-Range Biological Protonation Dynamics*

PC19 **Rožić, T.**: *Insights into non-statistical chemical reactivity from a vibrational relaxation model*

PC20 **Römer, A.**: *Theoretical studies of metal-metal cooperativity in pyrazolate-bridged complexes*

PC21 **Safy, M.**: *MACHO Catalyst for CO_2 to Methanol Conversion: A Computational Study of the Catalytic Mechanisms and Kinetics*

PC22 **Salamon-Krokosz, K.**: *Mechanistic studies of the fluorinated olefinic amino acid derivatives*

PC23 **Sawicki, I.**: *Impact of regularized second-order correlation energy expression on the Double Hybrid Functionals performance*

PC24 **Schnieder, B.**: *Quantum Chemical Study of the Combustion Reactions of Sulfur-Containing Char Systems using an Automatized Workflow*

PC25 **Schreder, L.**: *CASSCF wavefunctions embedded in a massively parallel Gaussian and plane waves density functional environment*

PC26 **Schürger, P.**: *Differential Shannon entropies characterizing electron-nuclear dynamics and correlation: Momentum-space versus coordinate-space wave packet motion*

PC27 **Seidenath, S.**: *Spicy ONIOMs: A New Implementation of Multi–Scale and Fragment Methods*

PC28 **Sen, A.**: *Identical Spin Multistate Reactivity Towards C-H Bond Activation in High-valent Mn/Fe-Oxo(Hydroxo) Species*

PC29 **Sharma, M.**: *Efficient Simulation of High Harmonic Generation Using Gaussian Basis Functions*

PC30 **Sharma, P.**: *Machine learning prediction of potential for surface hopping simulations, incorporating quantum vibrational effect*

PC31 **Shi, B.**: *Gold-Standard Wave-Function Methods Applied to Surface Adsorption*

PC32 **Singh, A.**: *Analyzing the limit for second-order correlation energy expression in the context of Adiabatic connection models*

PC33 **Skladanová, K.**: *Adsorption of benzene on graphene studied by ML-accelerated ab-initio molecular dynamics simulations*

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PC36 **Sukurma, Z.**: *Acceleration of the Auxiliary-Field Quantum Monte Carlo Procedure*

PC37 **Sun, Q.**: *Heterofission mechanism for pure organic room temperature phosphorescence*

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PC53 **Vörös, D.**: *Unveiling Surface Interactions of Push-Pull Functionalized Stilbene: Adsorption and Absorption on Silica Glass*

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