MONDAY

1. **Ajala,** Adeayo (Michigan State University)
"Recent Progress in the Electron-Attached, Ionized, and Active- Space Equation-of-Motion Coupled-Cluster Methodologies"

2. **Bauman,** Nicholas (Michigan State University)
"Coupled-Cluster Interpretation of the Photoelectron Spectra of Ag_3^- and Au_3^-"

3. **Bernales,** Varinia (University of Minnesota)
"Computationally Discovery of Active Decorated Metal-Organic Framework for Ethylene Oligomerization"

4. **Caricato,** Marco (University of Kansas)
"Evaluation of Electronic Coupling in Solids with DFT and PBC Calculations"

5. **Dandu,** Naveen (North Dakota State University)
"Effect of Surface Defects on Optoelectronic Properties of Thiol Functionalized CdSe Quantum Dots"

6. **Deustua,** J. Emiliano (Michigan State University)
"Benchmarking the Active-Space and Completely Renormalized Equation-of-Motion Coupled-Cluster Approaches for Vertical Excitation Energies"

7. **Gifford,** Brendan (North Dakota State University)
"The Electronic Properties of Finite Single Walled Carbon Nanotubes Capped with Different Functional Groups"

8. **Gurunathan,** Pradeep (Purdue University)
"Analytical Gradients for QM/EFP Dispersion Energy Term"

9. **Hégely,** Bence (Budapest University of Technology and Economics)
"Exact Density Functional and Wave Function Embedding Schemes Based on Orbital Localization"

10. **Horner,** Kate (Durham University)
"Magnetic Shielding Study of Urea-Based Gelators"

11. **Huang,** Chen (Florida State University)
"An Efficient and Robust Embedding Potential Solver for Density-Functional Embedding Simulations"

12. **Isayev,** Olexandr (University of North Carolina)
"Accurate Prediction of Properties for Inorganic Materials with Machine Learning"

13. **Jerabek,** Paul (CTCP Massey University)
"Understanding F 1s NEXAFS Dichroism in Perfluoropentacene"

14. **Karimova,** Natalia (Kansas State University)
"Time-dependent Magnetic Circular Dichroism of the Paramagnetic $Au_{25}(SC_2H_5)_{18}$ cluster"

15. **Khaliullin,** Rustam (McGill University)
"Fast Linear Scaling Density Functional Theory Based on Local Seamlessly Interconnected Orbital Domains"

16. **Kobayashi,** Masato (Hokkaido University)
"Fragmentation-Based Approach to Static Electron Correlation: Divide-and-Conquer Hartree–Fock–Bogoliubov Method"

17. **Lewis,** Cannada (Virginia Tech)
"O(N) Concentric Atomic Density Fitting: Accelerating Hartree- Fock Exchange Computation"

18. **Li,** Chenyang (Emory University)
"Driven Similarity Renormalization Group: Third-Order Multireference Perturbation Theory"

19. **Li,** Run (University of North Dakota)
"Parallelization of Triple and Quadruple Perturbed MRCI, nR-MRCISD(TQ), in UNDMOL"

20. **Manaa,** M. Riad (Lawrence Livermore National Laboratory)
"Enthalpies of Formation of Energetic Molecules with Composite Quantum Chemical Methods"

21. **McGreal,** Meghan (University of Minnesota)
"Computational Study of the Binding of H_2 in a FeNi Hydrogenase Active Site"

22. **Mihaylov,** Deyan (North Dakota State University)
"Multiple Exciton Generation in Semiconductor Nanostructures: DFT-based Computation"

23. **Morgenstern,** Amanda (Colorado School of Mines)
"Predicting Chemical Reactivity Using Gradient Bundle Condensed Fukui Functions"

24. **Muñiz,** Jesús (Universidad Nacional Autónoma de México)
"Benchmark Study on the Electronic Structure Properties of Polyoxometalate (POM) Keggin-like Structures at Carbon Substrates for Energy Storage Applications"

25. **Nagy,** Péter (Budapest University of Technology and Economics)
"Fragmentation-based Linear-scaling Electron Correlation Methods"

26. **Nanda,** Kaushik (University of Southern California)
"Calculating Non-linear Optical Properties of Closed- and Open-shell Species with EOM-CCSD: Theory and Examples"

27. **Ornellas,** Fernando (Universidade de São Paulo Instituto de Química)
"On the Electronic States of the Chromium Oxide Dication CrO^{2+}: A Theoretical Contribution"

28. **Parker,** Shane (University of California-Irvine)
"Unphysical Divergences in Response Theory"

29. **Patkowski,** Konrad (Auburn University)
"New Developments in Symmetry-adapted Perturbation Theory"

30. **Pearson,** John (Michigan State University)
"Grand Canonical Monte Carlo and Density Functional Theory Simulations of Flexible Metal Organic Frameworks"

31. **Podeszwa,** Rafał (University of Silesia)
"Crystal Structure Predictions from First Principles"

32. **Ramos-Cordoba,** Eloy (University of California-Berkeley)
"Excited States for Orbital-Optimized Second-Order Perturbation Theory"

33. **Rupnik,** Kresimir (Louisiana State University)
"Direct Measurements and Modelling of Electric Fields in Areas of Fundamental Significance to Bio-medicine: Ultra-High Magnetic Fields (UHMF)–Ultrafast Polarization Phase Selective Studies (UF PPS) at NHMF Laboratory"

34. **Rybkin,** Vladimir (ETH Zürich)
"Spin-Unrestricted MP2 Forces for the Condensed Phase: a Massively Parallel Implementation"

35. **Samu,** Gyula (Budapest University of Technology and Economics)
"Efficient Implementation of Three-center Coulomb-integrals and Their First Derivatives"

36. **Sun,** Qiming (Princeton University)
"PySCF: An Open Source Toolset Towards a Simple Electronic Structure Computation Environment"

37. **Tamukong,** Patrick (North Dakota State University)
"Properties and Nonadiabatic Dynamical Studies of Carrier Relaxation Rates in $Pb_{16}X_{16}/Cd_{52}Y_{52}$ (X, Y = S, Se, Te) Core/Shell Quantum Dots"

38. **Vogiatzis,** Konstantinos (University of Minnesota)
"Parallel CASSCF Calculations Beyond the Limits of the Conventional CASSCF Implementations"

39. **Wang,** Cong (Penn State University)
"General-order Spin-free Coupled Cluster Method: Generation and Simplification Using Permutation Group Techniques"

40. **Welden,** Alicia (University of Michigan)
"Thermodynamics from a Second Order Green's Function Method"

41. **Wen,** Xuelan (University of Minnesota)
"Projection-based Quantum Embedding Methods for Excited States"

42. **Zandkarimi,** Borna (University of Minnesota)
"Density Matrix Embedding Theory: Multi-Level Modeling of Complex Systems"

43. **Zech,** Alexander (University of Geneva)
"FDE-ADC: Multiscale Density Embedding With an Accurate Wavefunction Method"

TUESDAY

44. **Aebersold,** Lucas (Michigan State University)
"Density Functional Performance Utilizing Relativistic Effective Core Potentials for Lanthanide Compounds"

45. **Almora-Díaz,** César (UAM-Iztapalapa)
"Selected Configuration Interaction With Truncation Energy Error in Molecular Systems: Symmetric Dissociation of H_2O and Other Molecules"

46. **Anderson,** James (AICS, RIKEN)
"SR-ZORA Extension of QTAIM: Formulation and Examples"

47. **Aucar,** Gustavo (Natural and Exact Science Faculty UNNE and IMIT CONICET Argentina)
"Toward an Absolute NMR Shielding Scale Using the Spin-rotation Tensor Within a Relativistic Framework"

48. **Baskerville,** Adam (University of Sussex)
"Quantum Effects of Particle Motion in Atomic and Molecular Three-particle Systems"

49. **Boonseng**, Sarote (University of Sussex)
"The Formation of Pd(0) from Pincer Palladacycles"

50. **Borca**, Carlos (Purdue University)
"Exploring the Temporal Evolution of the Energy Components in the Effective Fragment Potential Molecular Dynamics"

51. **Bytautas** Laimutis, (Galveston College)
"Compact Description of Electron Correlation in Ab Initio Chemistry Using CI Wave Functions"

52. **Cárdenas**, Carlos (University of Chile)
"Chemical Response Functions in Degenerate States and Extended Systems"

53. **Chaves Claudino**, Daniel (University of Florida)
"Atomic Natural Orbital Basis Sets From Coupled-Cluster Density Matrices"

54. **De Wergifosse**, Marc (University of Southern California)
"Two-photon Absorption Spectra of Stilbene and Phenanthrene"

55. **Diaz**, Thomas (Michigan State University)
"Molecular Dynamics Simulations of the PKR Dimer"

56. **Doblhoff-Dier**, Katharina (Leiden University)
"Diffusion Monte Carlo for Accurate Dissociation Energies of 3d Transition Metal Containing Molecules"

57. **Fatehi**, Shervin (University of Texas Rio Grande Valley)
"Qualitative Criteria for Energy Transfer in Solution and Prospects for Research in the Fatehi Group at UTRGV"

58. **Gruber**, Thomas (Max Planck Institute for Solid State Research)
"Coupled Cluster Theory Studies of Phase Transitions in Solids and the Adsorption of Water on Solid Surfaces"

59. **Guo**, Sheng (Princeton University)
"Multireference Perturbation Theory Based on Density Matrix Renormalization Group"

60. **Hollett**, Joshua (University of Winnipeg)
"A Cumulant Functional for Static and Dynamic correlation"

61. **Humbert-Droz**, Marie (University of Geneva)
"Modelling the π Conjugation Length in Aromatic Antenna: A Simple Predictive Tool for the Synthesis of Functional Material"

62. **Jabed**, Mohammed (North Dakota State University)
"Photophysical and Electrochemical Properties of Small Silver Clusters Ligated by DNA-base Cytosine"

63. **Jin**, Yifan (University of Florida)
"Calculation of Core Electron Excitation Energies Using Optimized Density Functional Theory"

64. **Jones**, Michael (Michigan State University)
"Molecular Dynamics Simulations of the Asymmetric Dimer of the NF-κB Inducing Kinase"

65. **Jungong**, Akongnwi (University of North Dakota)
"Improving Far-UV CD Prediction with the Dipole Interaction Model"

66. **Kananenka**, Alexei (University of Michigan)
"Self-energy Embedding Theory"

67. **Karimova**, Natalia (Kansas State University)
"Time-dependent Magnetic Circular Dichroism of the Paramagnetic $Au_{25}(SC_2H_5)_{18}$ cluster"

68. **Kervazo**, Sophie (McMaster University)
"Relativistic Correlated Calculations of the Thermodynamics Properties of Gaseous Plutonium Oxides"

69. **Khaliullin**, Rustam, (McGill University)
"Covalency of Hydrogen Bonds in Liquid Water Can Be Probed by Proton Nuclear Magnetic Resonance Experiments"

70. **Kumar**, Chandan (University of Oslo)
"A New Response Theory Based Formulation of the Calculation of Nuclei-selected NMR Shielding Using Gauge-including Atomic Orbitals"

71. **Li**, Zhendong (Princeton University)
"Extensions of Ab Initio Density Matrix Renormalization Group"

72. **Magoulas**, Ilias (Michigan State University)
"Application of the CC(P;Q) Hierarchy of Coupled-Cluster Methods to the Challenging Problem of Be_2"

73. **Malbon**, Christopher (Johns Hopkins University)
"The Multichannel, Multistate Photodissociation of Hydroxymethyl Described Using a Coupled Quasi-diabatic Hamiltonian Fit to Accurate Ab Initio Data"

74. **Nohira,** Hiroyuki (Saitama University)
"Can Time-dependent Schrödinger Equation Accurately Describe the Time Evolution of Quantum States?"

75. **Patel**, Prajay (Emory University)
"Prediction of pKa for Late Transition Metal Hydrides Via a QM/QM Approach"

76. **Plascencia**, Cesar (Michigan State University)
"Correlation Consistent Composite Approaches for Transition Metal Complexes With Multireference Character"

77. **Reimann**, Sarah (University of Oslo)
"The Importance of Current Contributions to Shielding Constants in Density-functional Theory"

78. **Rivera-Arrieta**, Herzain (Universidad Nacional Autónoma de México)
"Structural Distortions Accompanying Non-Covalent Interactions"

79. **Rusakov**, Alexander (University of Michigan)
"Temperature-dependent Green's Functions and Electronic Correlations in Extended Systems"

80. **Shan**, Nannan (Kansas State University)
"First-Principles Insights into Furfural Electroreduction Pathways on Transition Metals"

81. **Skomorowski**, Wojciech (University of Kassel)
"Theoretical and Experimental Study of Penning Ionization Reaction at Very Low Temperatures"

82. **Tamukong**, Patrick (1) (North Dakota State University)
"Scalar Relativistic GVVPT2 Multireference Perturbation Theory Studies of Low-lying States of Mo_2 and Gd_2"

83. **Weerawardene**, Dimuthu (Kansas State University)
"Luminescence Properties of $Au_{25}(SR)^{1-}$ Nanoparticles"

84. **Winograd**, Blair (University of Michigan)
"A Stochastic Implementation of Second-order Green's Function Perturbation Theory"

85. **Yuwono**, Stephen (Michigan State University)
"Structural Optimization of Lanthanide Trihalides via Density Functional Theory"

86. **Senanayake,** Ravithree (Kansas State University)
"Theoretical Investigation of Electron and Nuclear Dynamics in the $Au_{25}(SH)_{18}^{-1}$ Thiolate-protected Gold Nanocluster"

87. **Reynolds,** Ryan D. (Northwestern University)
"Magnetic Properties from Fully Relativistic Theory: Zero-Field Splitting and the Pseudospin Hamiltonian"