#	Name	Title of presentation
1	**Pengchen Ma**	Mechanism studies in the De novo design of luciferases using deep learning
2	**Mojgan Asadi**	Understanding electrostatic effects in the function of biological systems
3	**Tatiana Mamani**	Oxygen Vacancy induced ferroelectric behavior in (111) SrTiO3 photoelectrodes for water oxidation
4	**Mitra Rooein**	Calculation of g-tensor and hyperfine coupling for photochromic copper complex
5	**James Shee**	Exploring new frontiers in transition metal quantum chemistry: Synergies between AFQMC, symmetry breaking, and CCSD(T)
6	**Liangyue (Willa) Wang**	Toward improved electrostatics in molecular dynamics: SMIRNOFF polarizabilities, bond charge corrections, and direct polarization
7	**Karnamohit Ranka**	Size-Dependent Errors in Real-Time Electron Density Propagation
8	**Frank Cerasoli**	High-throughput discovery of electron-precise clathrates and their superstructural ordering through machine learning
9	**Alexander Chang**	Understanding Biases within Reaction Discovery Methods using the ab initio Nanoreactor
10	**Jessica Flowers**	Beyond the Traditional Force Field: Improving IDP Conformer Sampling Through Dihedral Parameter Optimization
11	**Brianna Aguilar-Solis**	Approximating excited electronic states with spin-corrected self-consistent field methods
12	**Siddharth Sonti**	Elucidating the Fluxionality and Dynamics of Zeolite-Confined Au Nanoclusters Using Machine Learning Potentials
13	**Ilya Dergachev**	Modeling Quantum Tunneling in Nonadiabatic Statistical Theory
14	**Yuanheng Wang**	Ab Initio Interactive Molecular Dynamics with Accelerated Electron Repulsion Integrals
15	**Daria Nakritskaia**	Spin-vibrational resonances in molecular magnets in different environments
16	**Austin Atsango**	Machine-learned potentials capturing both aqueous excess protons and hydroxide ions for use with classical or quantum nuclei
17	**Brittany Harding**	Using the generalized thermal adiabatic connection to analyze and build exchange-correlation free energy approximations
18	**Martin Stoehr**	Adaptive Machine Learning-Assisted Semiempirical Quantum Chemistry
19	**Dean Lahana**	Competing Photochemical Decay Pathways in 2-bromothiophene
20	**Allen LaCour**	Predicting the Raman Spectra of Liquid Water from the Electric Field Distribution
21	**Bhaskar Rana**	Simulating the Excited-State Dynamics of Polaritons with Ab Initio Multiple Spawning
22	**Nicolas Sawaya**	Quantum algorithms for vibrational structure
23	**Andrew Snider**	Machine Learning Optical Spectra for Complex Chromophore Environments
24	**Selim Sami**	Advanced force fields guided by energy decomposition analysis
25	**Lukas Kim**	Learning a suitable bond index for reactive force fields
26	**Wenjun Xie**	Establishing the Evolution-catalysis Relationship for Enzymes to Reprogram Biocatalysis
27	**Imam Wahyutama**	Attosecond molecular charge migration simulations using the density matrix renormalization group
28	**Zhecheng He**	A binding model of C-peptide with BSA and Cu2+
29	**Anthony D. Dutoi**	Excitonic Renormalization for Large-scale Electronic-structure Calculations: Hermitian Variant
30	**Will DeSnoo**	Elucidating Palladium Catalyzed Allyl-Allyl Reductive Coupling Mechanism with H2 as Reductant
31	**Panyue Wang**	Water Prediction in the Tunnels of Respiratory Complex I
32	**Jesi Lee**	Modeling collision-induced-dissociation tandem mass spectrometry (CID-MS/MS) using ab initio molecular dynamics
33	**Andrew Bovill**	Characterizing Electronic Excited States Using Difference Density Natural Orbitals
34	**Bowen Han**	Incorporating Polarization and Charge Transfer into a Point-Charge Model for Water Using Machine Learning
35	**Yingze Wang**	iMiner workflow: A systematic physics-based machine learning workflow to propose drug molecules and evaluate the potency.

36	**Frank Hu**	Treating Semiempirical Hamiltonians as Flexible Machine Learning Models yields Accurate and Interpretable Results
37	**Amiel Stephen Paz**	Recovering dynamic correlation for SA-CASSCF with diabatic shifts: the diabatize-shift-diagonalize method
38	**Soren Holm**	Mechanochemical Reactivity of 2H-naphthopyran and Fluorinated Ladderane
39	**Cody Aldaz**	The Reaction Template Studio
40	**Maria Tsanai**	Investigating the interactions that drive the formation of biomolecular condensates
41	**Joseph Heindel**	Plausibility of Hydrogen Peroxide Production in Neutral and Charged Microdroplets
42	**Volga Kojasoy**	The Computational Investigation of the Role of Sulfur Noncovalent Interactions in the Thiopeptide Antibiotic Glycothiohexide Î±
43	**Nathan Yoshino**	Nanoreactor Studies of the Oligomerization of Diphosphorus to Red Phosphorus
44	**Jonathan Fajen**	Ab initio multiple spawning with coupled cluster singles and doubles for nonadiabatic dynamics of small organic molecules
45	**Srijan Bhattacharyya**	Disentangling timescale competition and topology to remove finite-size dependence in transport calculations
46	**Mingning Zhu**	Systematically Constructing the QM region for Excited States QM/MM Calculations
47	**Laura Weiler**	Efficient many-body expansion with GPU-acceleration and large fragments
48	**Christopher Myers**	The Interplay Between Solute-Solvent Interactions for Spectral Lineshapes of the Cresyl Violet Chromophore
49	**Rui Xu**	Reaction Discovery from First Principles: Bridging Ab Initio Molecular Dynamics and Kinetic Modeling for Methane Pyrolysis Experiment
50	**Eric Chung-Yueh Yuan**	Deep learning of nuclear Hessians: Beyond interatomic energies and forces
51	**Vsevolod Dergachev**	Calculation of non-adiabatic coupling with the crystal field Hamiltonian to predict spin relaxation in single-ion magnets
52	**Gilberto E. Fernandez**	Mechanism and Origins of Site-selectivity of Template-Directed C-H Insertion of Quinolines
53	**Colton Hicks**	Commoditizing Distributed Quantum Chemistry at Scale: BigChem and ChemCloud
54	**Tim Kowalczyk**	Electroactive 2D covalent organic framework design: insights from semiempirical simulation
55	**Shannon Houck**	Recent Advances In Q-Chem 6.1
56	**Maksym Fizer**	Analysis of diradical character in polysubstituted pentacenes
57	**Kevin Carter-Fenk**	Giving Time-Dependent Density Functional Theory X-ray Vision: Electron Affinity Approaches for Core-Excited States
58	**Kam-Tung (Tonybill) Chan**	A First-Principles Study of the Effect of Cations and Solvation Environment on the Solvation Shell and UV-Visible Absorption Spectra of a Nitrate Ion
59	**Diptarka Hait**	Nonradiative relaxation mechanisms for electronic excited states of radical ions
60	**Elisa Pieri**	In silico assessment of molecular photostability in cyclopentenones
61	**Jan Estrada Pabon**	Automated splitting of reactions paths for minimum energy path optimization
62	**Abdulrahman Y. Zamani**	Estimating vertical core excitation energies from Moller-Plesset theory with spin projection
63	**George Baffour Pipim**	Characterization of Oligo-p-phenylene Catalyst Used in CO2 Photoreduction: Conventional vs Range-Separated Hybrids
64	**Ethan Curtis**	Automated, Iterative Force Field Fitting
65	**Jason Tae Yi**	Narrow entrance to the quinone reaction chamber hinders water transfer in respiratory complex I
66	**Jie Li**	Highly Accurate Prediction of NMR Chemical Shifts from Cheap Quantum Mechanics Calculations Using Machine Learning
67	**Garrett Kukier**	Dissociation in Implicit Solvent
68	**Wentao Guo**	Unveiling the Mechanism of C-H Insertion combined Cope Rearrangement: Insights from Density Functional Theory and Ab Initio Molecular Dynamics Simulation
69	**Cristian Sarabia**	Computational Photophysical Characterization of Phenyl Pyrazine Ketones
70	**Pablo Andres Unzueta**	Resolving the Excited State Dynamics of Acetophenone