Young WATOC Saturday June 21

	SESSION ONE	*Chair: Abril Castro*		
08:45	**Opening**	Trygve Helgaker and Abril Castro		
09:00	Stefan Gugler	Technische Universität Berlin	Germany	Finding molecular minima and transition-states with reverse diffusion
09:20	Miguel Steiner	Massachusetts Institute of Technology	USA	Differentiable simulations for insight into multi-phase reaction mechanisms
09:40	Laura Grazioli	École nationale des ponts et chaussées	France	Excited states as critical points of the potential energy surface
10:00	Nina Glaser	University of Copenhagen	Denmark	Targeting Excited States on Early Fault Tolerant Quantum Computers
10:20	Frank Hu	Stanford University	USA	Accurate and efficient structure elucidation from NMR using artificial intelligence
	SESSION TWO	*Chair: Thomas Bondo Pedersen*		
11:10	Fabian Faulstich	Rensselaer Polytechnic Institute	USA	A static quantum embedding scheme based on coupled cluster theory
11:30	Marti Gimferrer	Georg-August-Universität Göttingen	Germany	On the impact of nuclear quantum effects in intermolecular interactions
11:50	Ji Woong Yu	Korea Institute For Advanced Study	South Korea	Investigation of anomalous water dynamics using machine learning force field
12:10	Madhubanti Mukherjee	École Polytechnique Fédérale de Lausanne	Switzerland	Exploring Additives for Crystallization of Halide Perovskites in Solar Cells
	SESSION THREE	*Chair: Michele Cascella*		
14:10	Marcos Casanova-Páez	Max-Planck-Institut für Kohlenforschung	Germany	Core-Excited States for Open-Shell Systems in Similarity-Transformed Equation-of-Motion Theory
14:30	Torsha Moitra	Comenius University in Bratislava	Slovaka	Real-time methods for light-induced attosecond spectroscopies
14:50	Ben McLean	RMIT University	Australia	Thermodynamics of graft copolymer self-assembly in mixed solvents: Molecular dynamics
15:10	Róża Okoń	Universitat de Barcelona	Spain	Small-molecule energy carriers for prebiotic metabolism models
15:30	Mariia Ivonina	Kyushu University	Japan	Decoding SARS-CoV-2 Pseudoknot Dynamics: Unraveling Drug Interaction Mechanism
	SESSION FOUR	*Chair: Ainara Nova*		
16:20	Rebecca Tomann	University Of California Berkeley	USA	Efficient Extended Tight Binding Implementation with Linear Scaling Algorithms
16:40	Leonardo Dos Anjos Cunha	Flatiron Institute	USA	Photonic observables and QEDFT functionals for strongly coupled light-matter systems
17:00	Sergio Moles Quintero	Vrije Universiteit Brussel	Belgium	Exploring Excited-State Aromaticity and Diradical Nature on Singlet Fission
17:20	Enric Petrus	EAWAG	Switzerland	Automated Exploration of Ozonation Reactions for Model Olefins in Water