The 7th ICReDD international symposium: The Rising Star Program

January 18th (Thursday)

8:30-9:00 Registration

9:10-9:20 Opening remarks

9:20-10:10 **David Bryce** (Department of Chemistry and Biomolecular Sciences, University of Ottawa, Canada)

"Modulation of Structure and Dynamics in Solids Featuring Non-Covalent s-Hole Interactions. An NMR Perspective"

10:10-10:40 **Koji Kubota** (Division of Applied Chemistry, Department of Engineering, WPI-ICReDD, Hokkaido Univeristy, JST-FOREST, Japan)

"*Exploring Mechanical Force-Induced Organic Synthesis*"

10:40-11:10 Coffee break

11:10-12:00 **Nobuhiro Yanai** (Department of Engineering, Kyusyu University, JST-CREST, Japan)

"Materials Chemistry for Optical Spin Polarization"

12:00-14:00 Lunch break

14:00-14:10 Session opening

14:10-14:40 **Midori Akiyama** (Graduate School of Science, Kyoto University, Japan)

"Perfluorocubane: A Novel Electron Acceptor Molecule"

14:40-15:05 **Yu Harabuchi** (WPI-ICReDD, JST-ERATO, Hokkaido University, Japan)

"Systematic exploration of reaction paths and non-radiative decay paths based on quantum chemical calculations toward chemical reaction discovery"

15:05-15:30 **Ruben Staub** (WPI-ICReDD, Hokkaido University, Japan)

"Accelerating reaction path search with Neural Network Potentials"

15:30-16:00 Coffee break

16:00-16:50 **Nong Artrith** (Debye Institute for Nanomaterials Science, Utrecht University, Netherland)

"Accelerated Sampling and Machine Learning Models for Non-Crystalline Energy Materials"

16:50-18:30 Poster session & reception

January 19th (Friday)

9:10-9:20 Opening remarks

9:20-10:10 **Julia Kalow** (Department of Chemistry, Northwestern University, USA)

"Harnessing Light for the Synthesis and Discovery of Optical Materials"

10:10-10:40 **Nobuya Tsuji** (WPI-ICReDD, Hokkaido University, Japan)

"Organocatalytic Asymmetric Hydrofunctionalizations"

10:40-11:10 Coffee break

11:10-12:00 **Yoichi Hoshimoto** (Osaka University, Japan)

"Exploring Ways to Harness N-Heterocyclic Carbenes and Triarylboranes in Organometallic and Synthetic Chemistry"

12:00-14:00 Lunch break

14:00-14:10 Session opening

14:10-15:00 **Ramil Nugmanov** (Johnson & Johnson Innovative Medicine, Belgium)

"Reactivity Modeling in Big Pharma"

15:00-15:30 **Pinku Nath** (WPI-ICReDD, Hokkaido University, Japan)

"Development of chemical ontology-based methodology to identify key features in chemical reaction dynamics"

15:30-16:00 Coffee break

16:00-16:50 **Philippe Schwaller** (Institute of Chemical Sciences and Engineering, Ecole Polytechnique Fédérale de Lausanne, Switzerland)

"Artificial Intelligence for Accelerated Chemical Synthesis"

16:50-17:00 Closing remarks