

# ICReDD/Hokkaido University Five Attached Institutes Joint Symposium

Bringing sciences together

March 7, 13:00-18:05, MON, 2022

Online  
No entry fee.

Opening remarks : 13:00-13:05 Kuniharu Ijiro (RIES)

<Session 1> 13:05-14:05 Chair : Jun-ya Hasegawa (ICAT)



• **Satoshi Maeda (ICReDD)**

"Artificial force induced reaction method: A computational approach for exploring chemical reactions based on quantum chemical calculations"



• **Takashi Toyao (ICAT)**

"Machine Learning for Heterogeneous Catalyst Design and Discovery"



• **Ronald Lazo Reyes (ICReDD)**

"Modularly Designed Supramolecular Catalytic Assembly for the Strategic Enantioselective Borylation of Remote C-H Bonds"

<Session 2> 14:15-15:15 Chair : Kenji Hirai (RIES)



• **Tetsuya Taketsugu (ICReDD)**

"Novel quantum chemical approach to chemical reactions: reduced-dimensionality reaction space and natural reaction orbital"



• **Naoki Watanabe (ILTS)**

"Negative Charge delivery in ice at 10 K: the role of surface OH radicals"



• **Vasudevan Pillai Biju (RIES)**

"Transient Charging and Charge Carrier Trapping in Semiconductor Nanocrystals"

<Session 3> 15:25-16:25 Chair : Kenji Iida (ICAT)



• **Tamiki Komatsuzaki (ICReDD)**

"Acceleration of Designing Chemical Reactions by Contextual Multi-armed Bandit Algorithm"



• **Yuki Ide (ICReDD)**

"Approaches to Construction of Chemical Reaction Image Diagnosis System Using Machine Learning"



• **Sheng Hu (ICReDD)**

"Data Representations for Deep Learning and Chemistry-Related Applications"

<Session 4> 16:35-17:55 Chair : Yuta Takano (RIES)



• **Hajime Ito (ICReDD)**

"Mechanochemical Organic Synthesis: A Revolution Platform"



• **Fumio Motegi (IGM)**

"Imaging the mechano-chemical feedbacks in biological patterning"



• **Manabu Igarashi (IIZC)**

"Structural bioinformatics studies of viral proteins"



• **Tetsuya Yamamoto (ICReDD)**

"Physics of gene regulation - Looking at genome from the viewpoint of soft matter physics and chemical reaction researches"

<Photo> 17:55-18:00

Closing remarks : 18:00-18:05 Satoshi Maeda (ICReDD)

