

Combination of Theoretical/Computational Studies and Experiments toward Porous Coordination Polymers/ Metal Organic Frameworks

Date: 22/08/2019

Place: Universitetet i Oslo, Kjemibygningen, Auditorium 3

program		
9:00-9:10	Opening remarks	Trygve Helgaker (University of Oslo)
Chair: Erik Tellgren (University of Oslo)		
9:20-10:00	A new approach to the multireference problem	Simen Kvaal (University of Oslo)
10:00-10:40	Theoretical Approaches for Coordination Asymmetry: Photoreaction in MMF and Chiroptical Spectroscopy	Masahiro Ehara (Institute for Molecular Science)
10:40-11:00	Coffee break	
11:00-11:40	Computational design of multivariate MOFs for CO₂ conversion to methanol	Ainara Nova (University of Oslo)
11:40-12:20	Theoretical Study of Infinite System Consisting of Transition Metal Complex	Shigeyoshi Sakaki (Kyoto University)
12:20-13:50	Photo & Lunch	
Chair: Michiko Atsumi (University of Oslo)		
13:50-14:30	Zr-MOFs at UiO: Recent advances in synthesis and postsynthetic methods	Sigurd Øien-Ødegaard (University of Oslo)
14:30-14:50	Functionalisation of UiO-67	Gurpreet Kaur (University of Oslo)
14:50-15:10	Coffee Break	
15:10-15:30	Decoration of Crystal Surface of PCPs/MOFs and Control of Their Porous Properties	Ken-ichi Otake (Kyoto University)
15:30-16:10	Dynamic Properties of Soft PCPs / MOFs	Susumu Kitagawa (Kyoto University)
16:10-16:20	Closing remarks	Michiko Atsumi (University of Oslo)