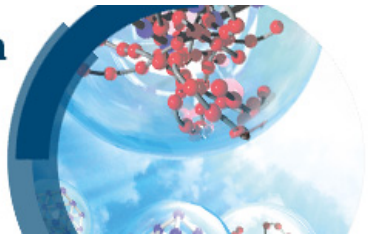
Cooperative phenomena in framework materials

Faraday Discussion



13-16 October 2020
Online

Please note all times in BST

Tuesday 13 October 2020

13:00	**Welcome and Introductions** *Susumu Kitagawa and François-Xavier Coudert, co-Chairs of Scientific Committee*
13:10	**Outline of Discussion Format** *Caroline Knapp and Kirsten Hall, Royal Society of Chemistry Publishing Editors*
13:15	**Introductory Lecture** (Session Chair: Susumu Kitagawa) Omar Farha *Northwestern University, United States*
14:15	**Close of sessions**

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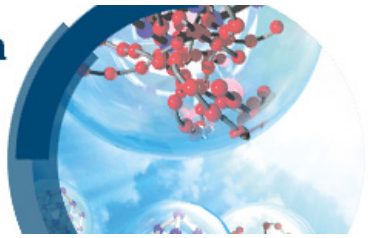

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Wednesday 14 October 2020

	Session 1: Advanced characterisation techniques: multi-scale, in situ, and time-resolved (Session Chair: Christian Doonan)
08:00	**Molecular motion in the nanospace of a MOF upon gas adsorption investigated by in situ Raman spectroscopy** Ryotaro Matsuda *Nagoya University, Japan*
08:05	**MOF Matrix Isolation: Cooperative Conformational Mobility Enables Reliable Single Crystal Transformations** Christopher Sumby *University of Adelaide, Australia*
08:10	**Exploring cooperative porosity in organic cage crystals using in situ diffraction and molecular simulations** Samantha Chong *University of Liverpool, UK*
08:15	Discussion
09:15	Break
	Session 2: Materials breaking the rules (Session Chair: Masako Kato)
09:45	**The role of temperature and adsorbate on negative gas adsorption in the mesoporous metal-organic framework DUT-49** Simon Krause *University of Groningen, Netherlands*
09:50	**Cooperative phenomenon of vapochromism and proton conduction of luminescent Pt(II) complexes for visualization of macroscopic proton conduction pathway** Atsushi Kobayashi *Hokkaido University, Japan*
09:55	**Face-selective adsorption of a prochiral compound on the chiral pore-surface of metal-macrocycle framework (MMF) directed towards stereoselective reactions** Shohei Tashiro *The University of Tokyo, Japan*
10:00	Discussion
11:00	Break
	Session 1 Continued: Advanced characterisation techniques: multi-scale, in situ, and time-resolved (Session Chair: Stefan Kaskel)
11:30	**Can 3D Electron Diffraction Provide Accurate Atomic Structures of Metal-Organic Frameworks?** Zhehao Huang *Stockholm University, Sweden*
11:35	**Multi-stimulus linear negative expansion of a breathing $M(O_2CR)_4$-node MOF** Lee Brammer *University of Sheffield, UK*
11:40	Discussion
12:40	Lunch break
	Session 2 Continued: Materials breaking the rules

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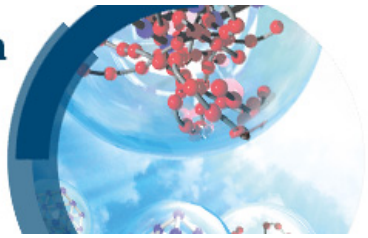

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	(Session Chair: Stefan Kaskel)
13:40	**Identifying the liquid and glassy states of coordination polymers and metal–organic frameworks** Thomas Bennett *University of Cambridge, UK*
13:45	**Trends in the Thermal Stability of Two-Dimensional Covalent Organic Frameworks** William Dichtel *Northwestern University, United States*
13.50	**Function from configurational degeneracy in disordered frameworks** Andrew Goodwin *University of Oxford, UK*
13.55	Discussion
14:55	**Poster Session 1**
15:55	**Close of Sessions**

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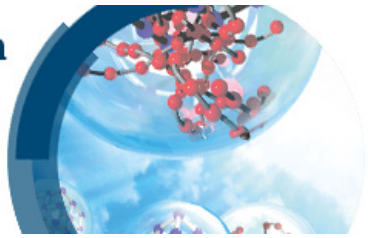

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Thursday 15 October 2020

	Session 3: Novel Computational Tools (Session Chair: François-Xavier Coudert, Masako Kato (part 2))
08:00	**The micromechanical model to computationally investigate cooperative and correlated phenomena in metal-organic frameworks** Sven Rogge *Ghent University, Belgium*
08:05	**Cooperative and synchronized rotation in motorized porous frameworks: Impact on local and global transport properties of confined fluids** Jack Evans *TU Dresden, Germany*
08:10	Discussion
08:50	Break
09:20	**Atomistic insight in the flexibility and heat transport properties of the stimuli-responsive metal-organic framework MIL-53(Al) for water-adsorption applications using molecular simulations** Veronique Van Speybroeck *Ghent University, Belgium*
09:25	**Influence of Flexible Side-Chains on the Breathing Phase Transition of Pillared Layer MOFs: A Force Field Investigation** Rochus Schmid *Ruhr-Universität Bochum, Germany*
09:30	Discussion
10:10	**Poster Session 2**
11.10	**Close of Sessions**

	Session 4: Towards complex systems and devices (Session Chair: François-Xavier Coudert)
13:00	**Exploring the Dynamics of Zr-Based Metal-organic Frameworks Containing Mechanically Interlocked Molecular Shuttles** Benjamin Wilson *University of Windsor, Canada*
13:05	**Photoelectrochemical Alcohol Oxidation by Mixed-Linker Metal-Organic Frameworks** Amanda Morris *Virginia Tech, United States*
13:10	**Adsorber heat exchanger using Al-fumarate beads for heat-pump application – a transport study** David Farrusseng *CNRS, France*
13.15	Discussion
14:15	**Close of Sessions**

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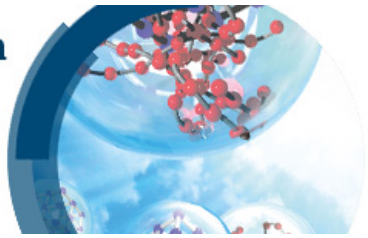

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Friday 16 October 2020

	Session 4: Towards complex systems and devices (Session Chair: Christian Doonan)
08:00	**Crystal Melting and Vitrification Behaviors of the Three-Dimensional Nitrile-Based Metal–Organic Framework** Satoshi Horike and Chinmoy Das *Kyoto University, Japan*
08:05	**Inclusion of viologen cations leads to switchable metal-organic frameworks** Andrew Burrows, Laura Cadman and Mary Mahon *University of Bath, UK*
08:10	**Discussion**
08:50	**Closing remarks** Jianwen Jiang *National University of Singapore*
09:30	**Acknowledgements** *Scientific Committee*
09:40	**Close of Meeting**

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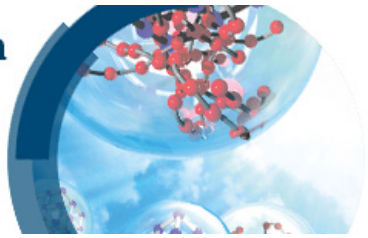

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