Furukawa Group Seminar

Date

July 25th, 2024
10:30–12:00

Venue

Kyoto University, KUIAS
iCeMS Main Building

2F Seminar Room
(#A207)

Registration

· Required from Google form
(https://forms.gle/h1mzDmC92UvH1KNw7)

· On-site only

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In situ insights into adsorption and catalysis in Metal-Organic Frameworks

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Abstract

To develop and optimize novel adsorbents that exhibit selective metal-adsorbate interactions or specific guest adsorption, and to thoroughly characterize their crystal structure, electronic, and oxidation/charge states, it is essential to elucidate the role of coordinatively unsaturated metal centers, specific adsorption sites, and key physical changes upon guest binding. To this aim, the combination of *in situ* and *operando* crystallographic and spectroscopic techniques is becoming essential for understanding the structure-function relationships of metal-organic frameworks (MOFs) demonstrating that a multi technique approach can uncover unprecedented details about the underlying processes.

My research group focuses on understanding the structural changes in long-range order and local environments during adsorption processes and catalysis. We utilize *in situ* X-ray diffraction and *operando* X-ray absorption experiments, or a combination of both. Our work includes synthesizing novel adsorbent MOF materials, rationalizing gate-opening effects and cooperative gas adsorption phenomena, and identifying key active sites during adsorption and catalysis.

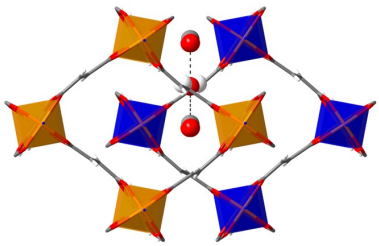
In this lecture, I will present our recent findings, achieved through a combination of advanced techniques, including custom-made setups. Key studies to be discussed include: i) *in situ* detection of specific adsorption sites for CO_2 adsorption under humid conditions; ii) Combined XAS/PXRD experiments to describe the evolution of long-range and local structures during adsorption experiments; iii) in-depth analysis of 'PXRD CO_2 adsorption isotherms', encompassing the retrieval of heat of adsorption and host-guest interactions through ab-initio structure solution and Rietveld methods.

References

[1] L. Braglia; F. Tavani; S. Mauri; R. Edla,; D. Krizmancic; A. Tofoni; V. Colombo; P. D'Angelo; P. Torelli *J. of Phys. Chem. Lett.* 12, 37, 9182 (2021).

[2] R. Vismara; S. Terruzzi; A. Maspero; T. Grell; F. Bossola; A. Sironi; S. Galli; J.A.R.; V. Colombo *Adv. Mater.* 2209907 (2023).

[3] A. Tofoni; F. Tavani; M. Vandone; L. Braglia; E. Borfecchia; P. Ghigna; D. Stoian; T. Grell; S. Stolfi; V. Colombo; P. D'Angelo *J. Am. Chem. Soc.* 145, 38, 21040 (2023).



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