Furukawa-Kitagawa Group SEMINAR

"Molecular level resolution of defects in MOFs and their catalytic activity"

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Thursday November 7th, 2019 11:00-12:00
Kyoto University KUIAS (iCeMS Main Building)
2F Seminar Room (#A207)

In this talk I will discuss work on our group which encompasses several distinct topics: water ice, zeolites, MOFs, condensed matter and novel boron chemistry. However, for most of the talk I will focus on metal organic frameworks and how we use state of the art modelling approaches to elucidate structure and reactivity of MOFs. MOFs have transitioned from materials with "promise" to commercial, niche products. While existing applications are chiefly in the molecular storage/delivery and molecular separation areas, there is considerable interest in the potential for MOFs to perform catalysis. Arguably the most promising material in this field is UiO-66 and related Zr_6 block-based structures such as NU-1000. It has been known for some time that defects in these materials facilitate catalysis; at least two such types of defect have been inferred: missing linker and missing cluster. An open question has been which defect is more active? In recent work[1], we have identified ordered defects, using imaging combined with calculations to rationalize the mechanism of crystal growth in this material. Moreover, we have identified that missing clusters appear to be more active for one test reaction, although specific reactions might be facilitated by missing linkers. In this talk, I will discuss recent efforts to shed light on the driving force for ordering of defects and the acidity differences in the different defects to try and rationalize why these defects facilitate reactivity.

References: L. Liu et al., Nature Chemistry, 11, 622-628 (2019)

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