

On the interaction of guest molecules with Co-MOF-74: A Vis/NIR and Raman approach

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Co-MOF-74 rod like crystals with a length of several hundred micrometers have been synthesized via a solvothermal procedure and their interaction with different gases has been evaluated in view of selective gas sensing. We show strongly anisotropic absorption behaviour of the Co-MOF-74 crystals when illuminated with polarized light. This study then addresses the interactions of guests (CO₂, propane, propene, Ar, MeOH, H₂O) with Co-MOF-74, studied by various spectroscopic techniques. Via Vis/NIR measurements, peak shifts of Co-MOF-74 depending on the interaction with the guest molecules were observed and distinguished. In the visible as well as in the near infrared region, the maximum absorbance is shifted selectively corresponding to the intensity of the Co^{II}-guest interaction. Even propene and propane could be distinguished at room temperature according to their different interactions with Co-MOF-74. Furthermore, we used Raman spectroscopy to detect a modified vibrational behaviour of Co-MOF-74 upon gas adsorption. We show that the adsorption of H₂O leads to a characteristic shift of the peak maxima in the Raman spectra.

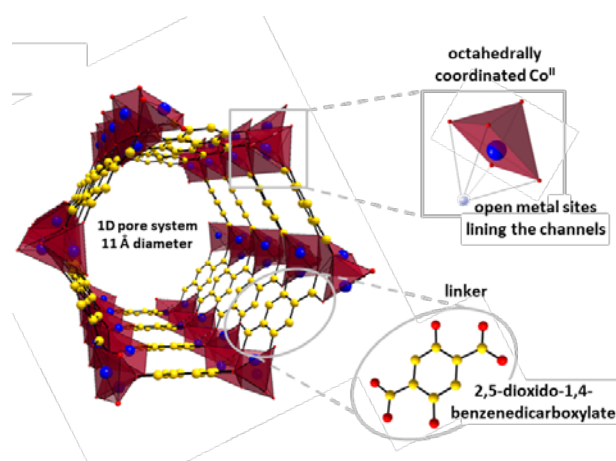


Figure 1. Crystal structure of Co-MOF-74, octahedrally coordinated Co^{II} with open metal sites lining the interior of the pore, and the organic linker 2,5-dioxido-1,4-benzenedicarboxylate

Summarizing, we were able to demonstrate the strongly anisotropic absorption behavior of Co-MOF-74 crystals illuminated by polarized light. Afterwards Co-MOF-74 has been evaluated for selective gas sensing. Several gases (CO₂, propene, propane, Ar, MeOH, H₂O) can be detected and distinguished by Co-MOF-74 due to their interactions with the Co²⁺ centers. We detected different peak shifts in the Vis/NIR spectra which could be correlated with the metal-guest interaction. Guests like propene, CO₂, MeOH and H₂O show a stronger interaction with the Co^{II} metal-centers than propane and Ar. In case of propene, an interaction of the Co^{II} with the double bond is assumed, for CO₂ one oxygen atom is interacting with the metal center and in case of MeOH and H₂O the molecules interact via their oxygen atom and can additionally develop hydrogen bonding between the hydrogen atoms of H₂O or MeOH and the oxygen atoms of the organic linker.

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