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Combinatorial design and structural characterization of sulfur containing 3D imine COFs

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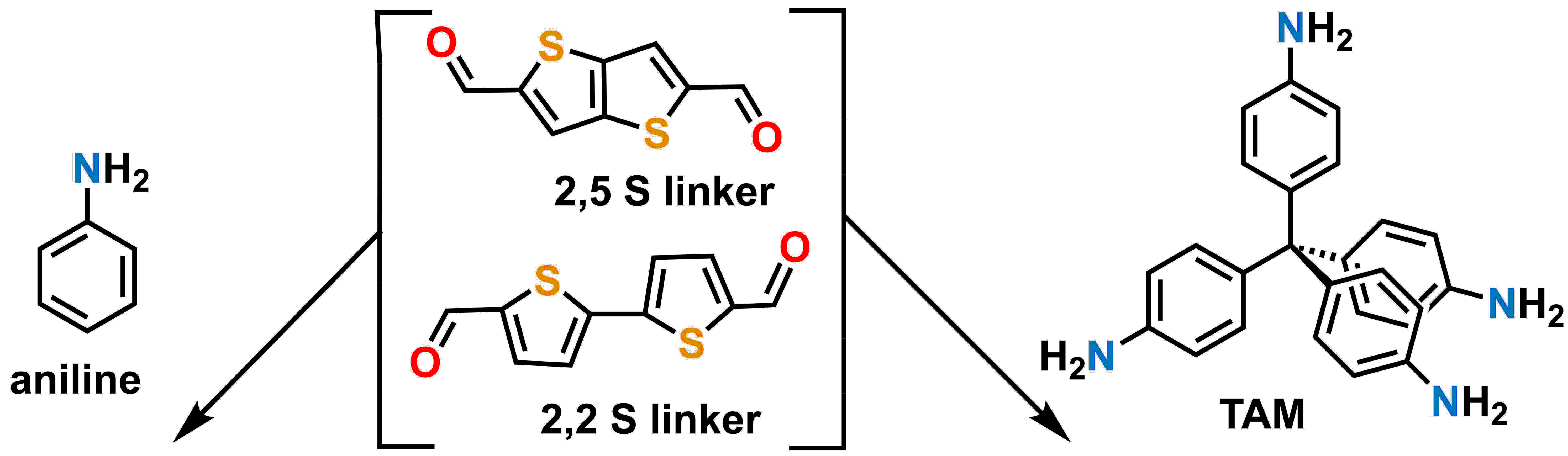
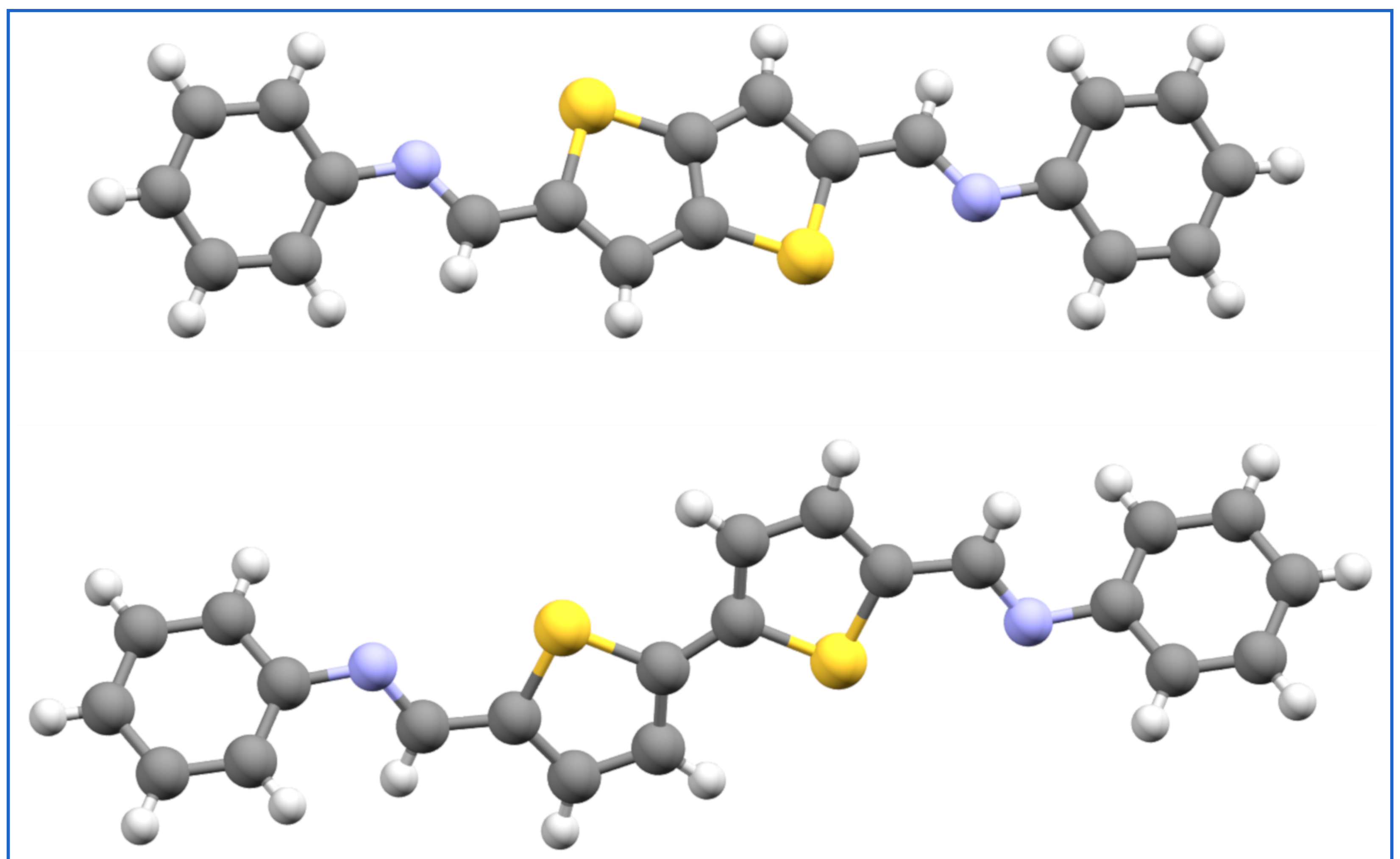
Introduction

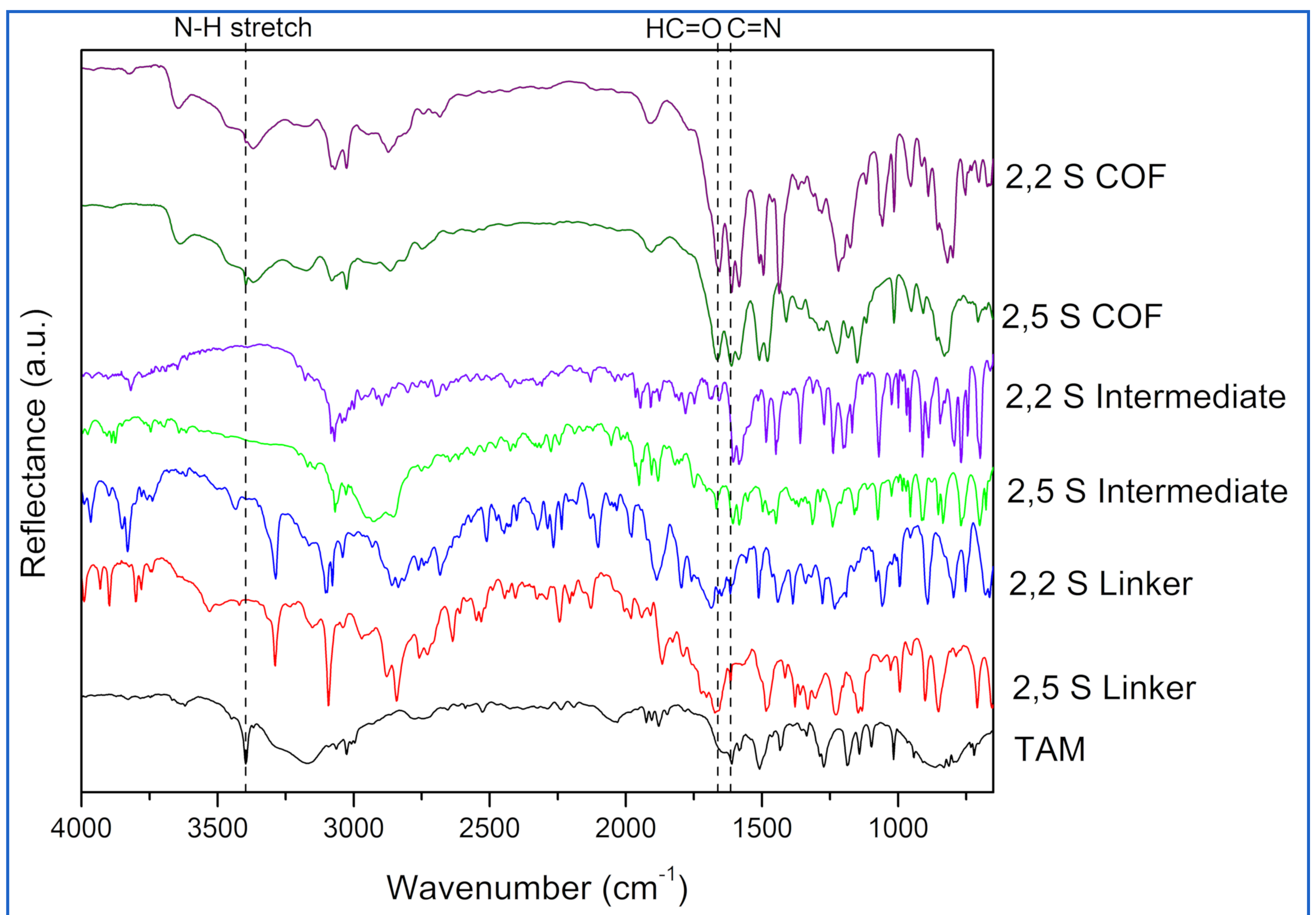
While a lot of effort has been put in the design and synthesis of imine linked Covalernt Organic Frameworks (COFs), reports of 3D structured materials are still quite scarce, owing to the specific linker geometry required to obtain fully interconnected 3D networks. [1] Therefore, it could be of high interest to develop novel functionalized 3D Covalent Organic Frameworks. In this project, we combined two sulfur bearing aldehyde linkers with the commonly used 3D COF building block TAM, to obtain sulfur containing 3D COFs. To the best of our knowledge, this is the first report of sulfur bearing 3D Covalent Organic Frameworks.



Intermediates suitable for SXRD

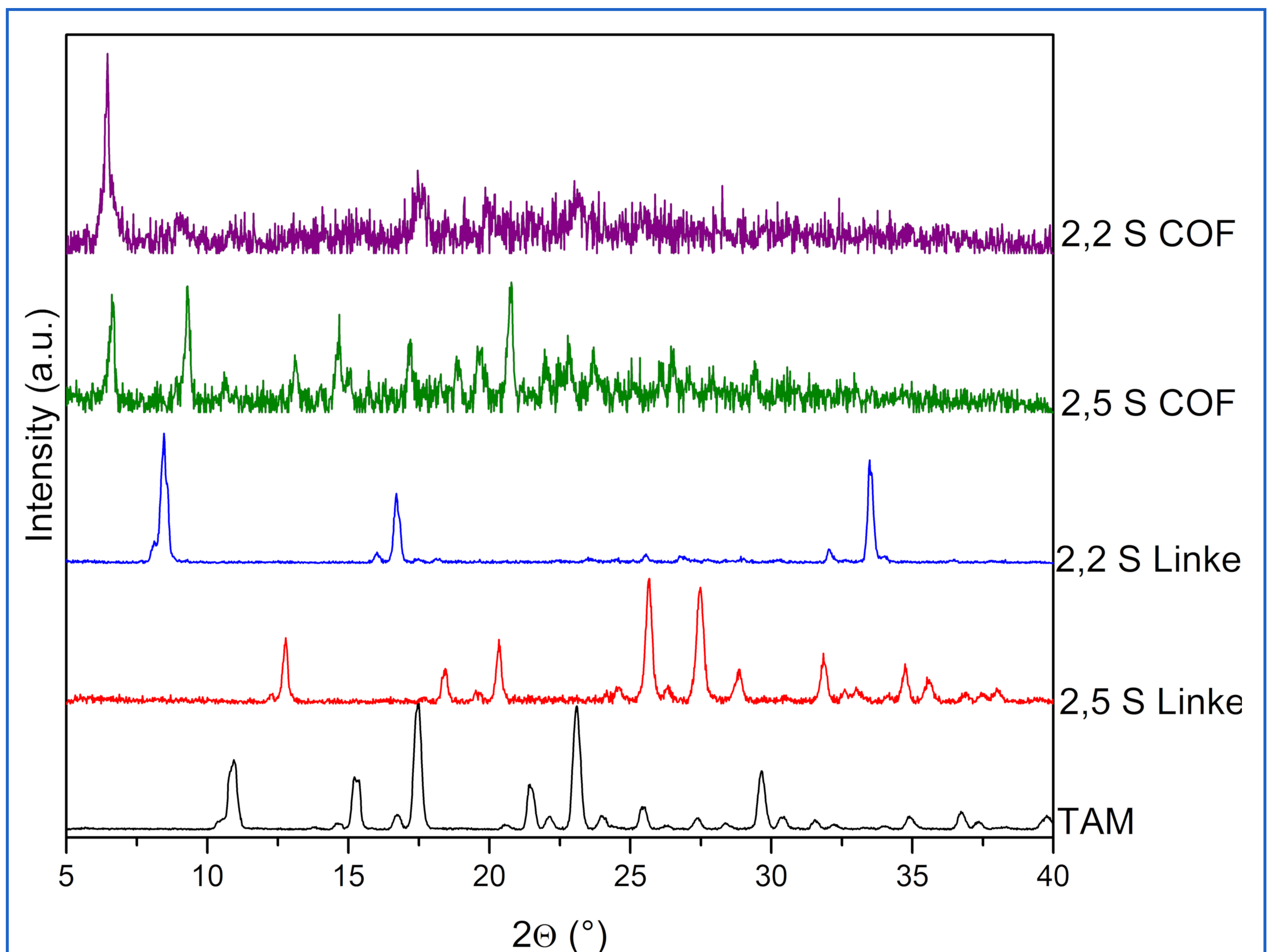


Analysis of the intermediates using Single Crystal X-Ray Diffraction showed close proximity of the sulfur atoms to the imine nitrogens, creating an environment suitable for metalation of the COF materials.

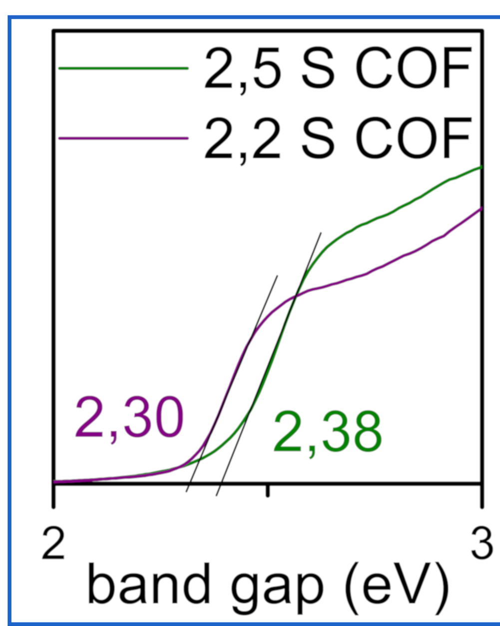


Using FTIR spectroscopy, the formation of COF was confirmed by the appearance of an imine band . However, the partial elimination of starting materials suggested incomplete reaction with remaining aldehyde and amine functions in the COF material.

S containing 3D COFs



Crystallinity of the samples was confirmed via Powder X-Ray Diffraction. For both materials, two characteristic COF peaks, very comparable to COF 300s hydrated and dehydrated diffraction peaks [2], could be observed around 6.5 and 9° 2θ. Even after thorough cleaning, a peak belonging to residual TAM could be distinguished in both samples.



The band gap of the materials was estimated via solid state UV-VIS spectroscopy. As expected, the band gaps of both materials are very comparable and situated in the visible range (quite close to green light). This makes them potentially attractive for use as metal-free photocatalysts.

Future Scope & Conclusions

Two crystalline, 3D sulfur containing COFs were succesfully prepared and characterized. These materials will be tested as catalysts in a range of photocatalytic metal-free reactions. Furthermore, to increase understanding and knowledge of the materials, we will try to prepare crystals suitable for Single Crystal X-Ray Diffraction.

[1] O. M. Yaghi, M. J. Kalmutzki, C. S. Diercks, *Introduction to Reticular Chemistry: Metal-Organic Frameworks and Covalent Organic Frameworks*, Wiley - VCH, Weinheim (Germany), **2019**, Chapter 9, 238.
[2] D. M. Fischbach, G. Rhoades, C. Espy, F. Goldberg, B. J. Smith, *ChemComm*, **2019**, 55, 3594.

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