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TOWARDS ROBUST METAL-ORGANIC FRAMEWORKS BASED ON FLUORINATED LINKERS FOR GAS STORAGE

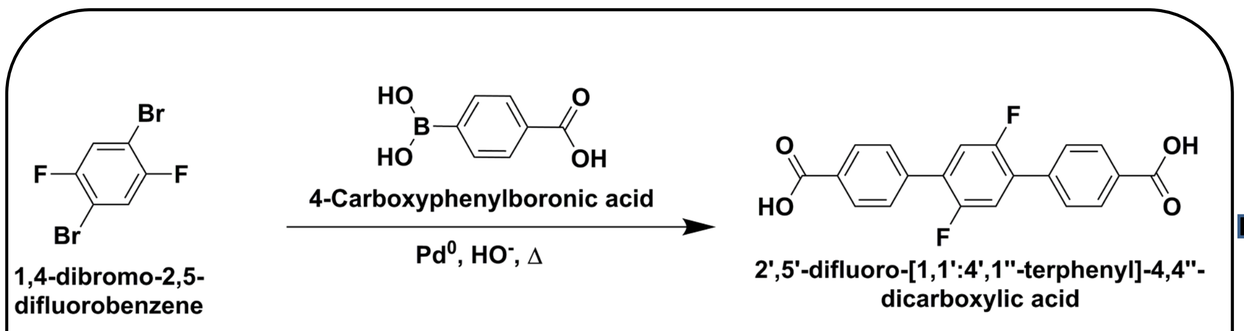
Ioan-Andrei Dascălu, Sergiu Shova, Rodinel Ardeleanu, Narcisa Marangoci, Mariana Pinteală, Christoph Janiak

[1] *Petru Poni Institute of Macromolecular Chemistry, 41A Aleea Gr. Ghica Voda, Iaşi 700487, Romania*

[2] *Institute for Inorganic and Structural Chemistry, Heinrich-Heine University Dusseldorf, 40225 Dusseldorf, Germany.*

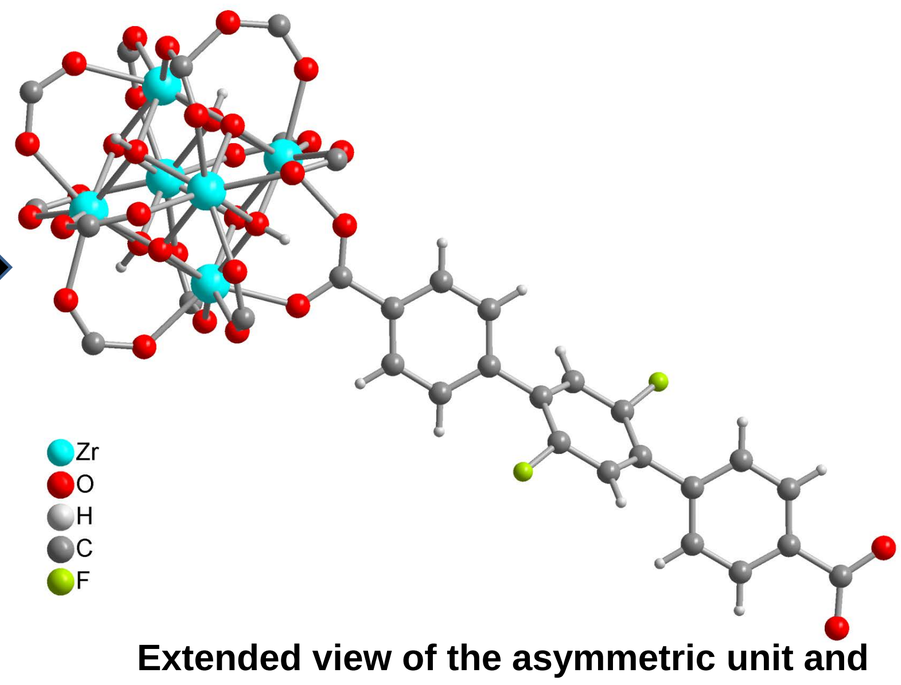
**E-mail of the main author: idascalu@icmpp.ro*

Metal-organic frameworks MOF are an intensely studied class of materials owing to their porous nature that have found use in applications such as gas storage and separation, catalysis, water adsorption, etc. These compounds are three dimensional networks comprised of metal nodes interconnected by rigid organic molecules called linkers. The developments of a new MOF for a specific application, apart from selecting the coordinating metal, involves the selection of the linker features such as size, shape, number and nature of coordinating groups or the presence of specific functional groups. This report describes the development of a fluorous zirconium MOF starting with the preparation of the ligand 2',5'-difluoro-[1,1':4',1''-terphenyl]-4,4''-dicarboxylic acid through a one-step reaction.

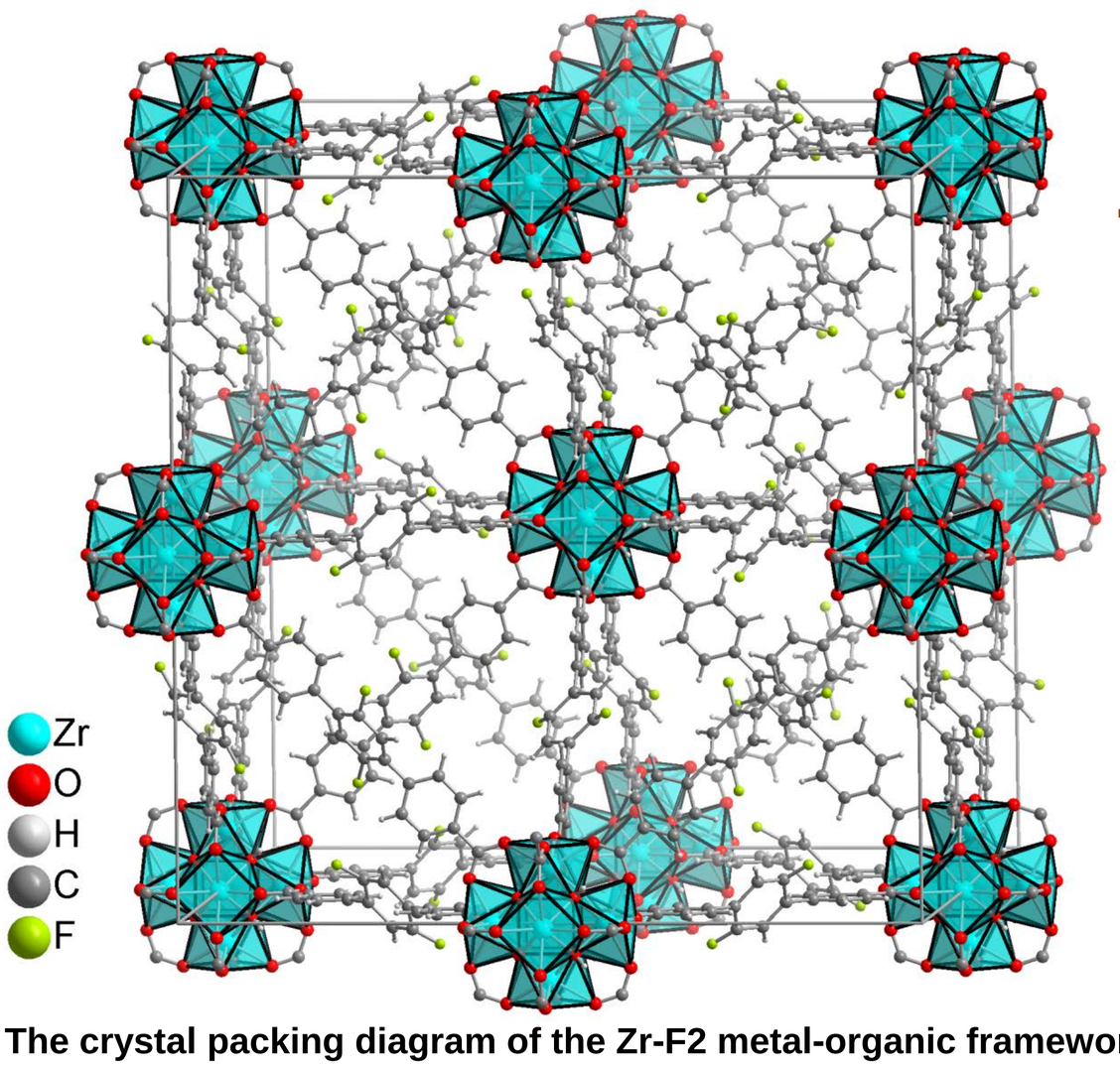


One-step synthesis procedure of the ligand 2',5'-difluoro-[1,1':4',1''-terphenyl]-4,4''-dicarboxylic acid (H2F2).

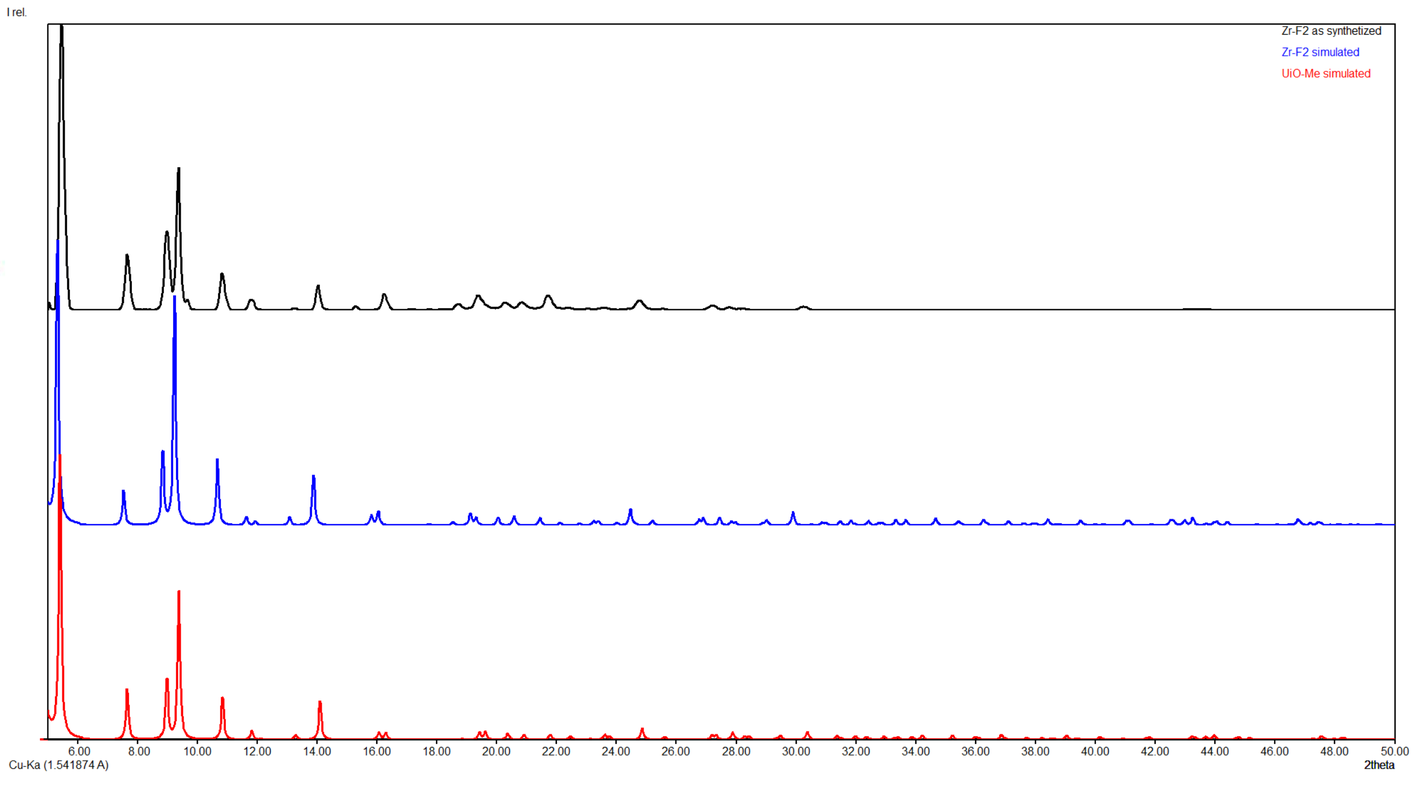
$ZrCl_4$,DMF
CH_3COOH
120°C



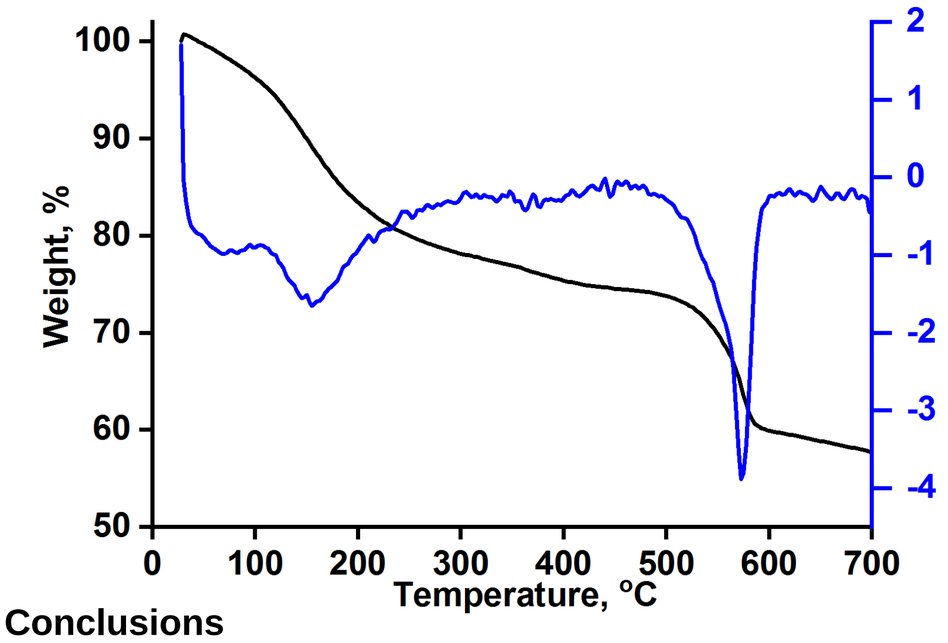
Extended view of the asymmetric unit and coordination environment around Zr in the metal-organic framework Zr-F2



The crystal packing diagram of the Zr-F2 metal-organic framework.



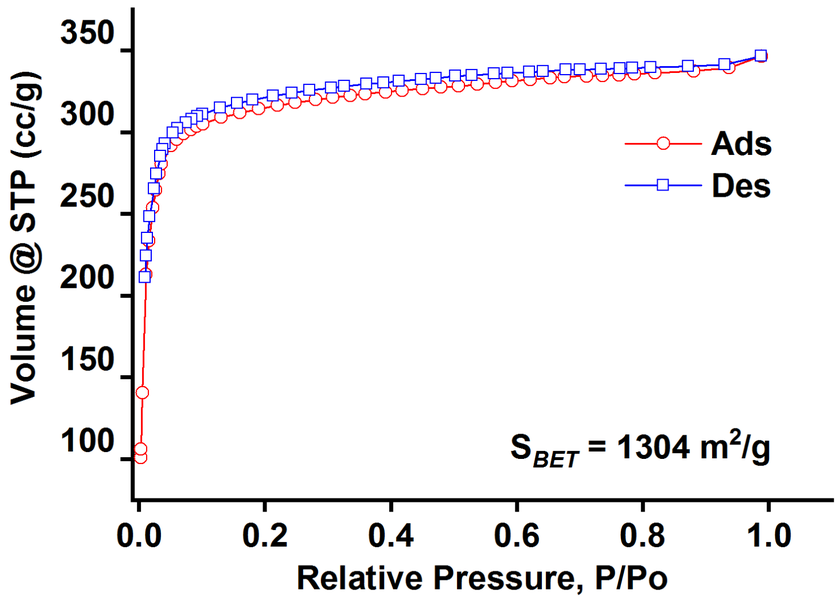
X-ray powder diffraction pattern of the measured Zr-F2 MOF sample compared to the theoretical UiO-68 and Zr-F2 diffractograms.



Thermal analysis

Zr-F2 metal-organic framework

Nitrogen sorption isotherms



Conclusions

The synthesis and purification procedure for a therphenylic linear dicarboxylic acid has been achieved. The partially fluorinated linker was successfully used in the preparation of a robust zirconium metal organic framework. The detailed structure and phase purity of the 3D network was demonstrated by single crystal and powder X-ray diffraction. The obtained MOF demonstrated high thermal stability (~400 °C) and a BET surface area of approximately 1300 m^2/g. This design strategy will be exploited in MOF synthesis experiments with linkers functionalized with a various number of fluorine atoms.

Acknowledgements

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