# Mechanical Properties of Melt-Quenched MOF Glasses and Their Relation to Microstructure – Will the Neutron Scattering be the Key Tool?

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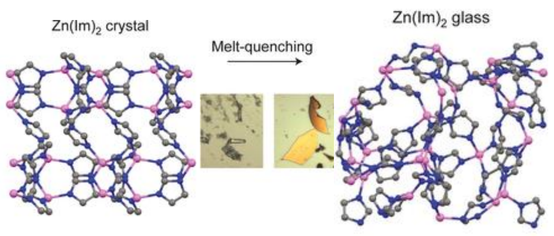
## Introduction

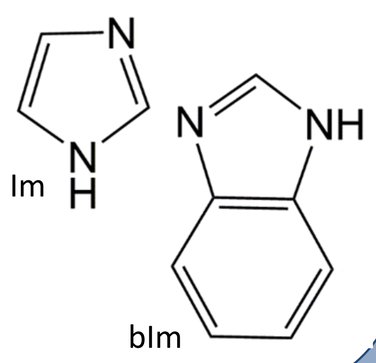



- Metal-organic frameworks are hybrid materials composed of inorganic nodes and organic linkers.
- One of the subsets: ZIF (**Zeolitic Imidazolate Frameworks**).
- It was recently shown that it is possible to vitrify some ZIF crystalline materials by heating up over $T_m$ and rapid cooling [1-3].

**How does chemical composition affect properties of MOF glasses?**

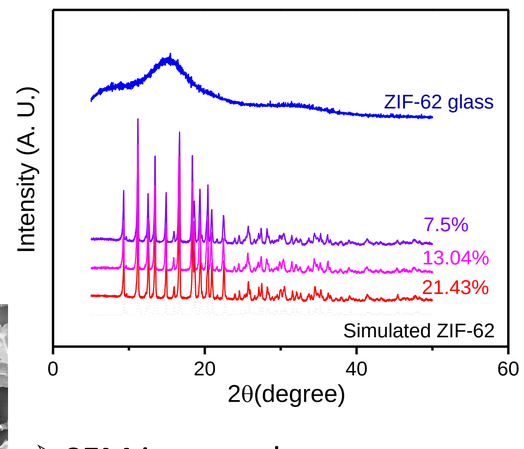
We focus on ZIF-62: zinc nodes connected with two different types of ligands: imidazole (Im, $C_3H_4N_2$) and benzimidazole (bIm, $C_7H_6N_2$).

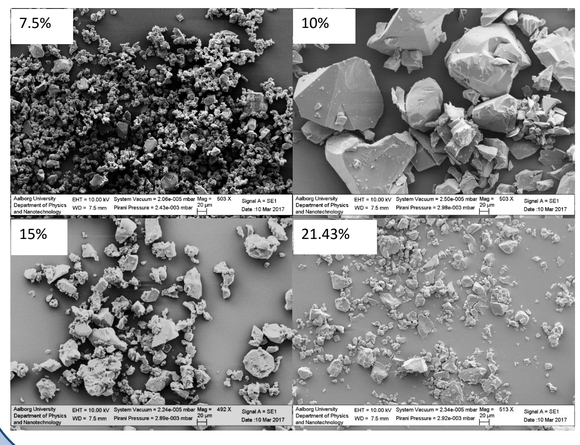
By changing the ratio of ligands during synthesis we study how they influence properties of obtained material.




## Synthesis of crystalline ZIF-62 with changing ligand ratio

- Synthesized crystals contained from 7.5% to around 21.5% benzimidazole.
- Powder XRD was preformed in order to ascertain all obtained crystals were ZIF-62.

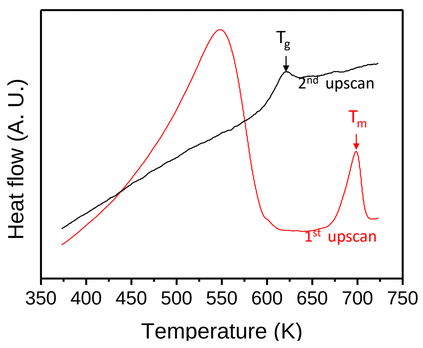


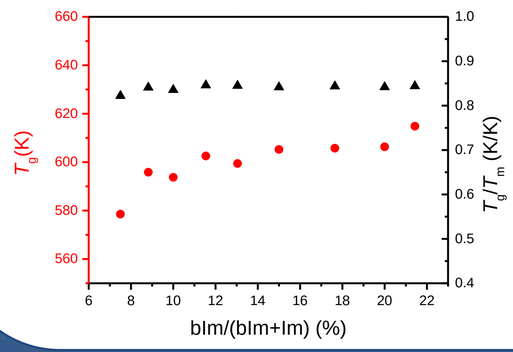

- SEM images show most crystals are of similar size, but those containing 10% bIm – characterized by much larger crystal size.

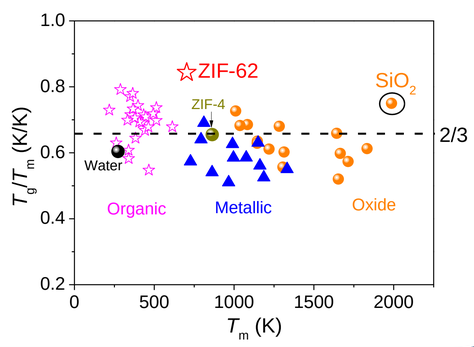
## Vitrification and thermal response

- Second upscan shows glass transition peak, Indicating ZIF-62 is vitrified.
- Glass transition temperature ($T_g$) increases with increasing benzimidazole.



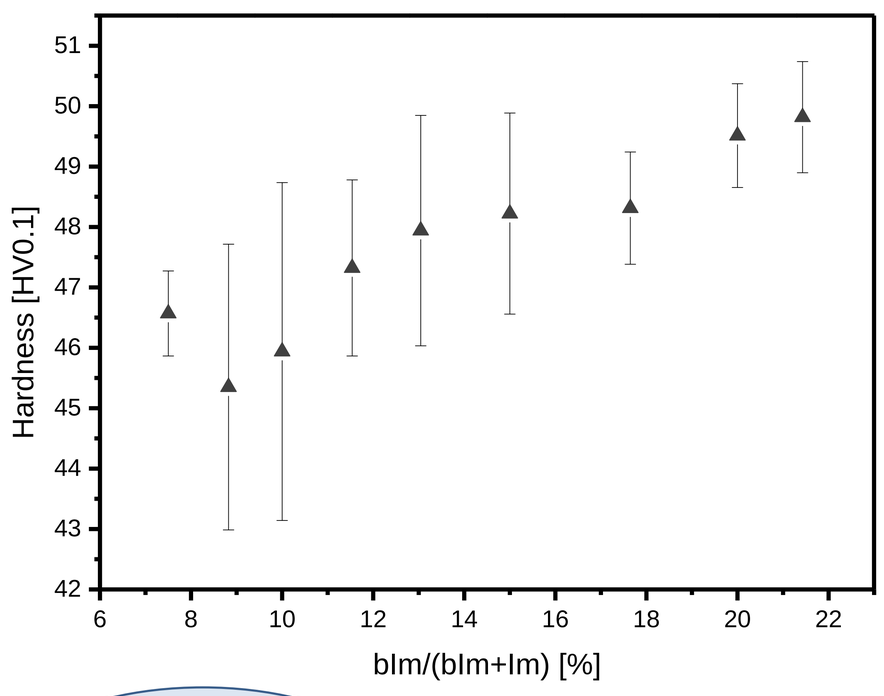

- $T_g/T_m$ is high compared to most glassy materials.




## Mechanical properties

**An increase of hardness is visible when increasing benzimidazole content:**



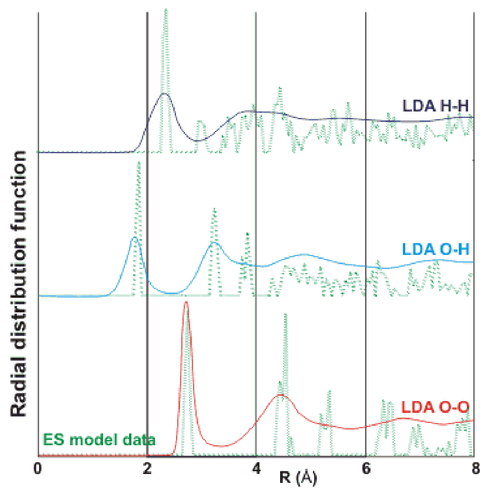

Uncertainty is relatively high – needs to further confirm by additional tests.

Possible source of the error:
- Chemical inhomogeneity;
- Porosity;
- Processing;
- Instrument accuracy.

## Why neutron scattering?

**To gain deeper insight into structure-properties relations.**

- The technique is sensitive for detecting the response of the structure to change of chemical composition, temperature, time...
- It is extremely important for us to characterize the light atoms in organic ligands.




Source: [4]

## Conclusion

- Changing the ratio between two different organic ligands influences mechanical properties of ZIF-62 glass.
- The next step is to understand the structural changes. We need sensitive measure – such as neutron scattering.

## References

[1] T. D. Bennett, J.-C. Tan, Y. Z. Yue, et al., *Nat. Commun.*, 2015, **6**, 8079.
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[4] M. C. Bellissent-Funel, J. Teixeira and L. Bosio, *J. Chem. Phys.* **87** (1987) 2231-2235.
[5] M. Stepniewska, C. Zhou, Y. Z. Yue, to be submitted.