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Stepniewska, Malwina; Zhou, Chao; Yue, Yuanzheng

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

Malwina Stepniewska, Chao Zhou, Yuanzheng Yue

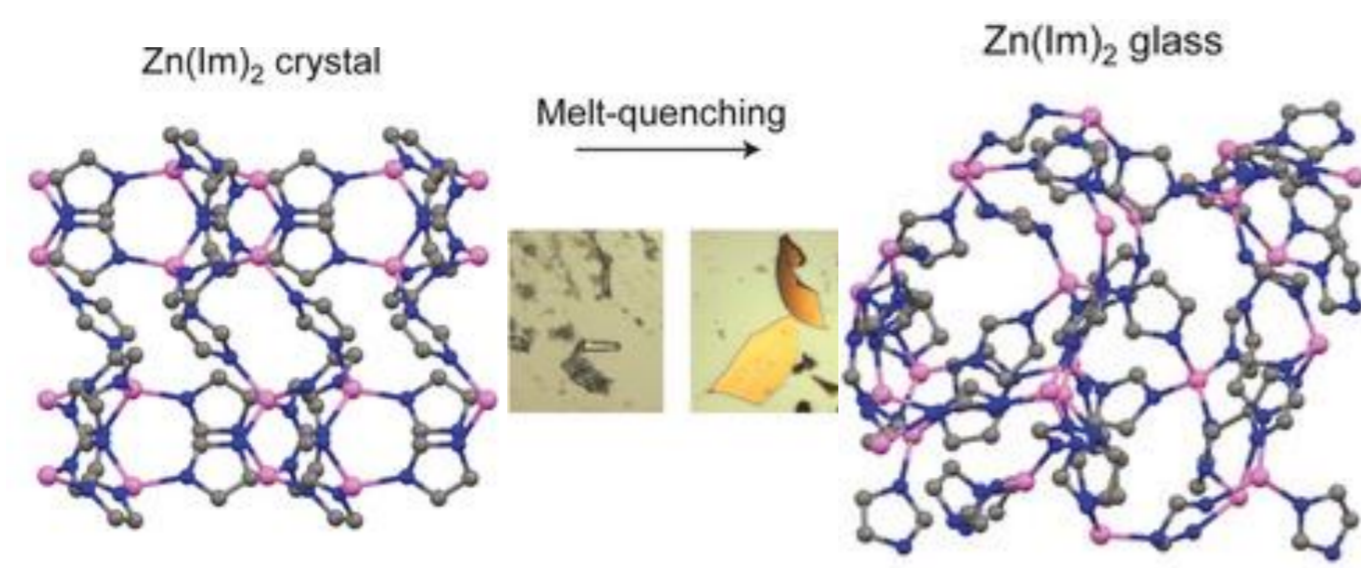
Department of Chemistry and Bioscience, Aalborg University, DK-9220 Aalborg, Denmark

Corresponding author: mst@bio.aau.dk

Introduction

➤ Metal-organic frameworks are hybrid materials composed of inorganic nodes and organic linkers.

➤ One of the subsets: ZIF (Zeolitic Imidazolate Frameworks).

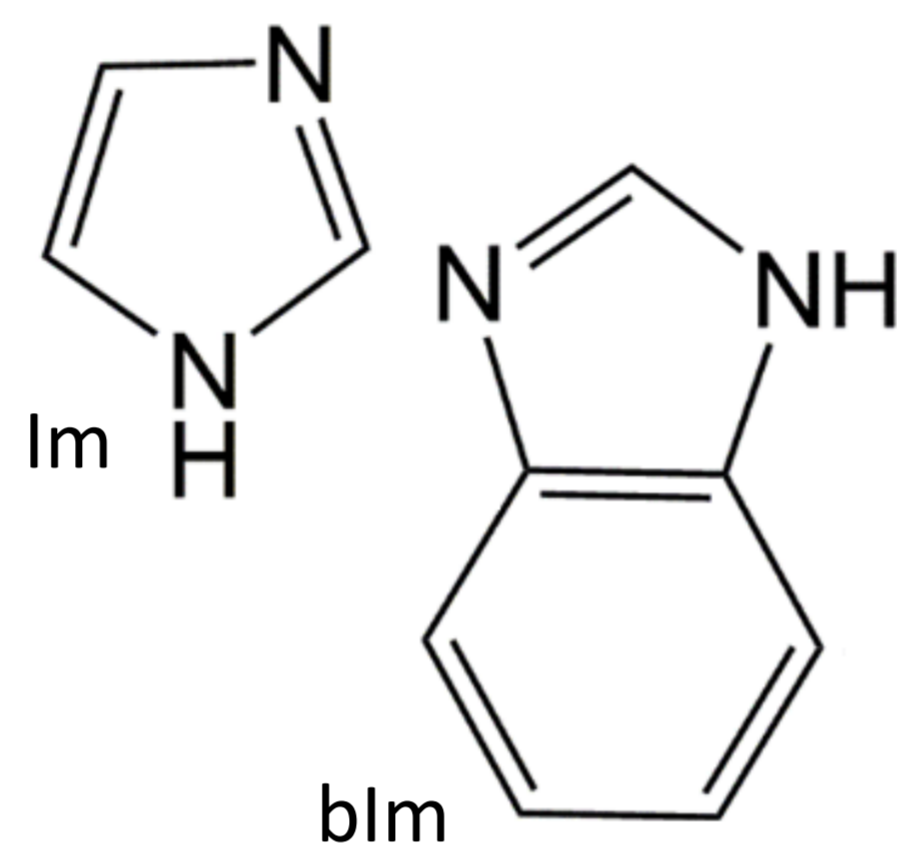


➤ It was recently shown that it is possible to vitrify some ZIF crystalline materials by heating up over T_m and rapid cooling [1-3].

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 (blm, $C_7H_6N_2$).

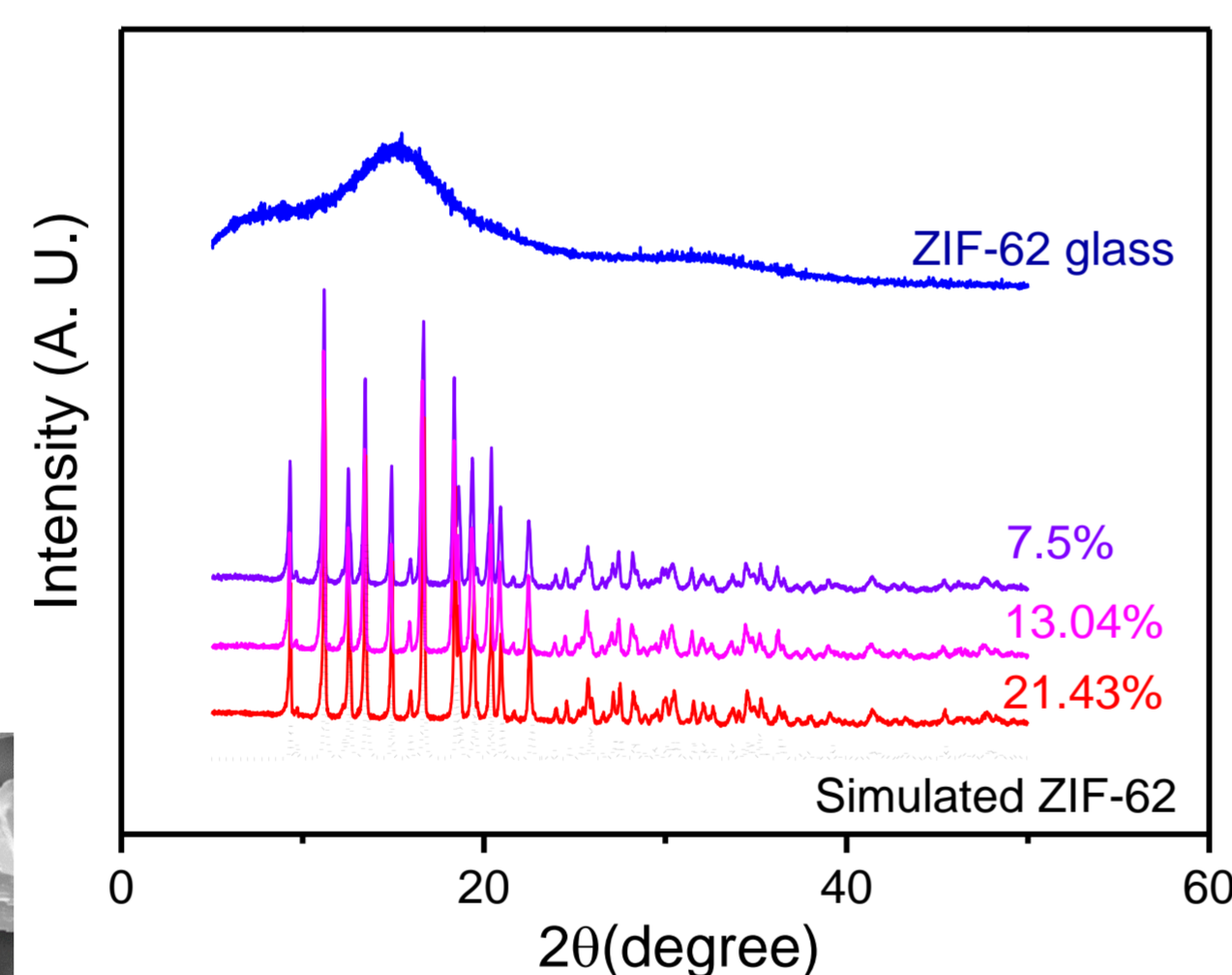
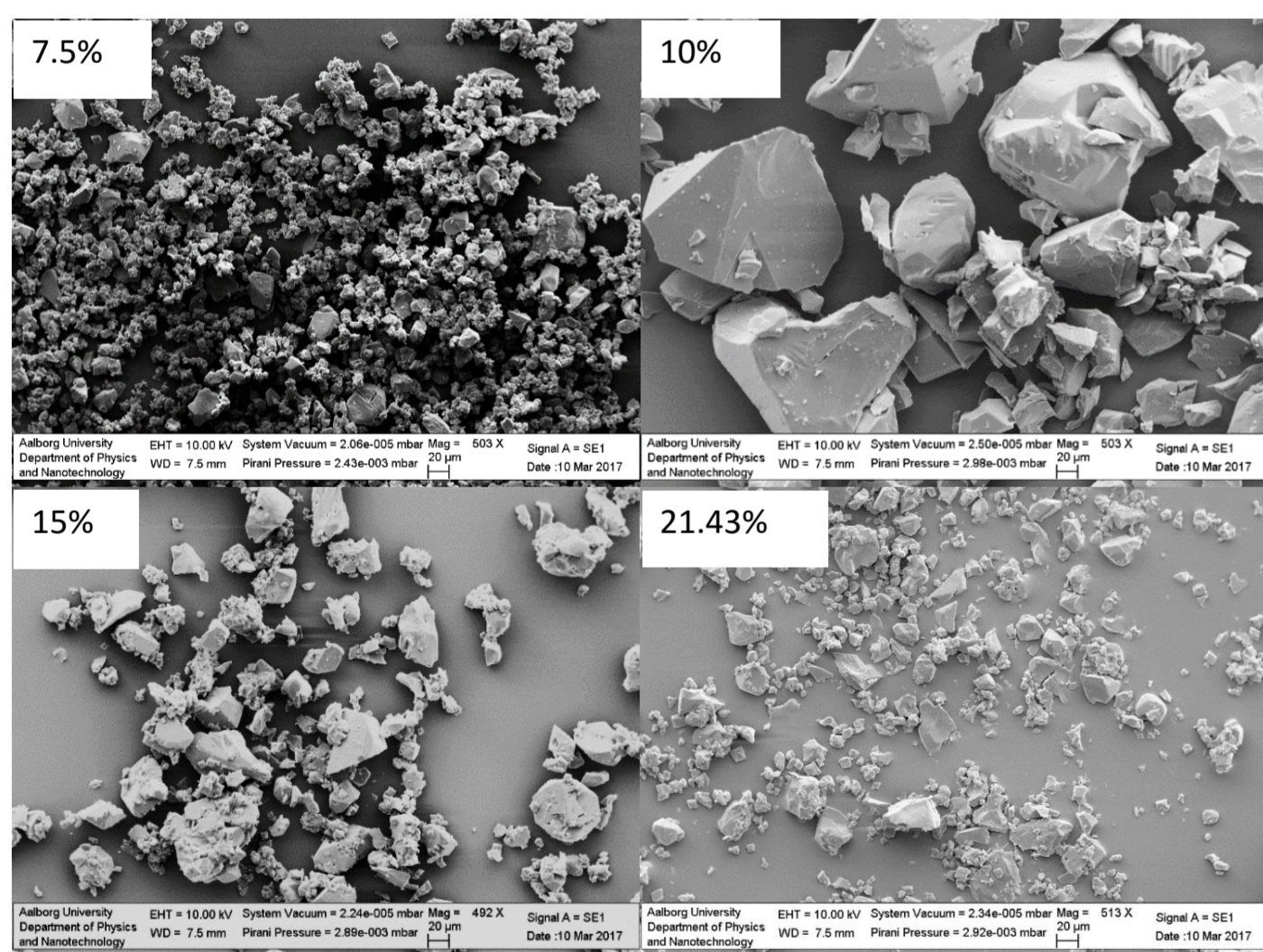
By changing the ratio of ligands during synthesis we study how they influence properties of obtained material.



Synthesis of crystalline ZIF-62 with changing ligand ratio

➤ Synthesized crystals contained from 7.5% to around 21.5% benzimidazole.

➤ Powder XRD was performed in order to ascertain all obtained crystals were ZIF-62.



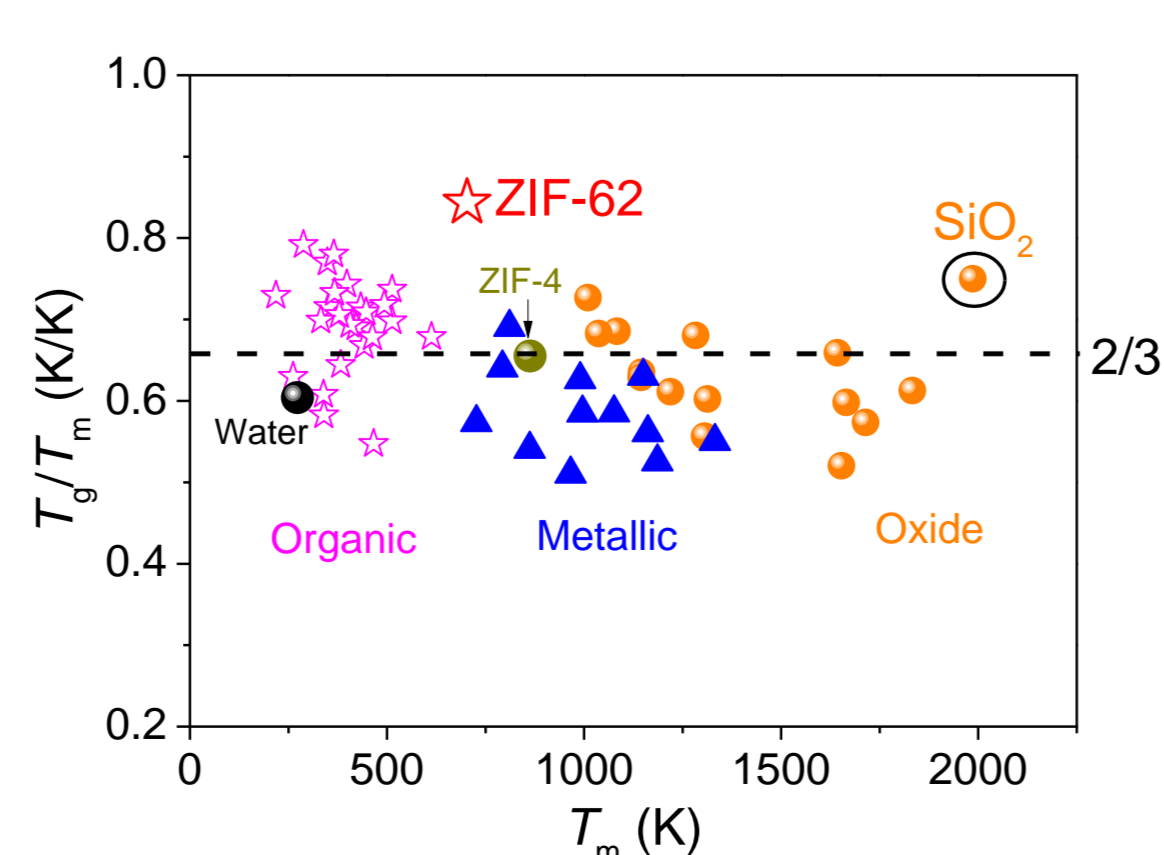
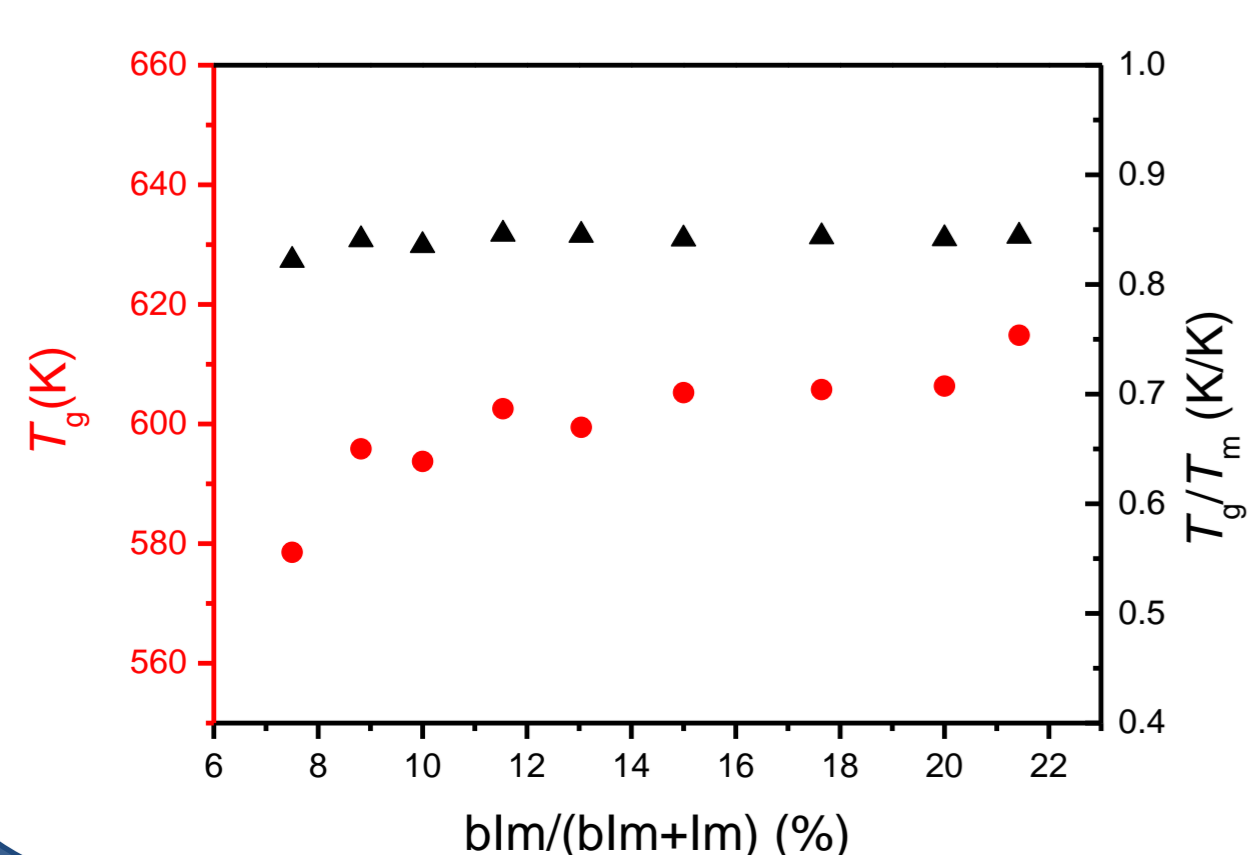
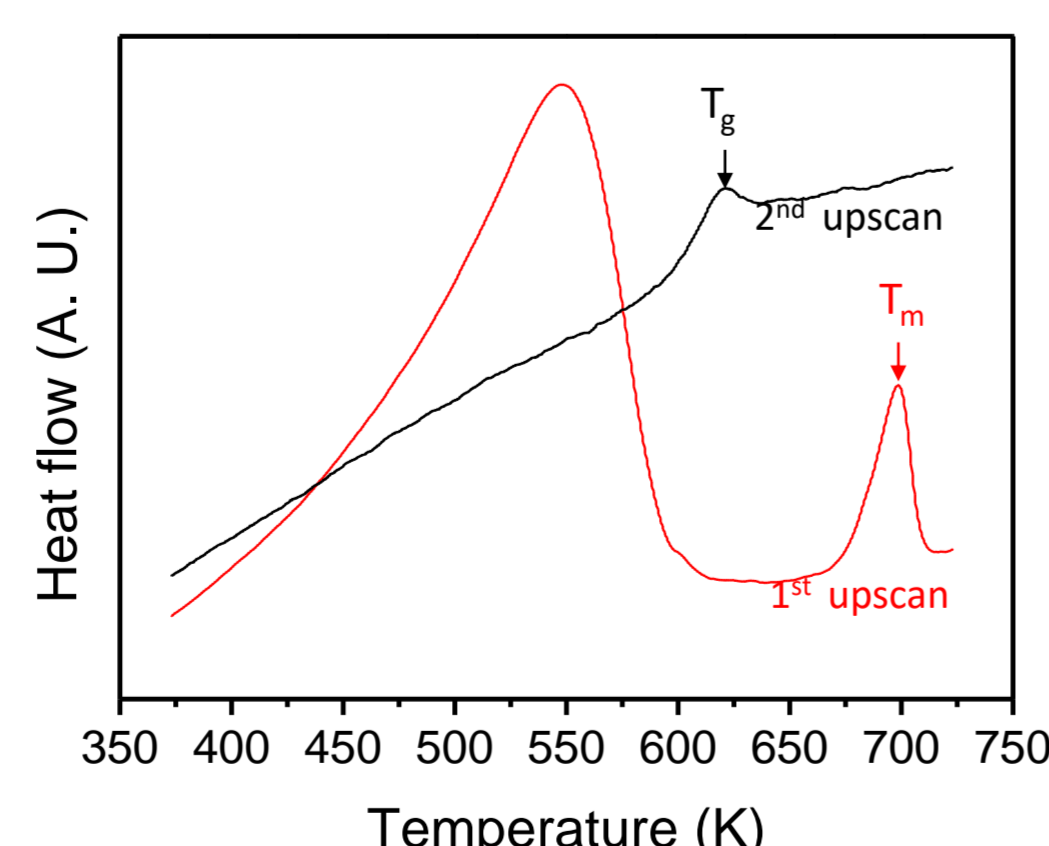
➤ SEM images show most crystals are of similar size, but those containing 10% blm – characterized by much larger crystal size.

Vitrification and thermal response

➤ Second upscan shows glass transition peak, indicating ZIF-62 is vitrified.

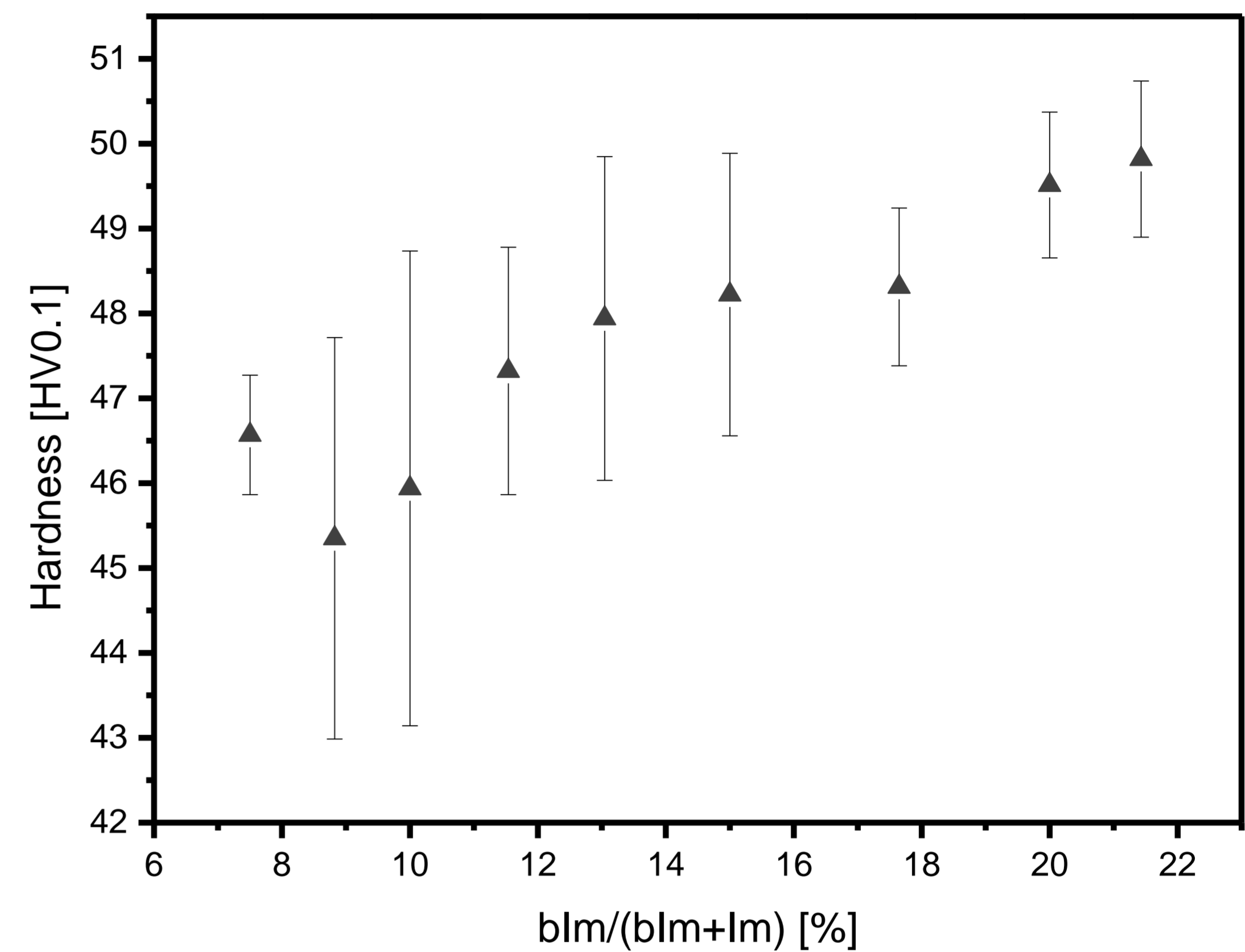
➤ Glass transition temperature (T_g) increases with increasing benzimidazole.

➤ 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:

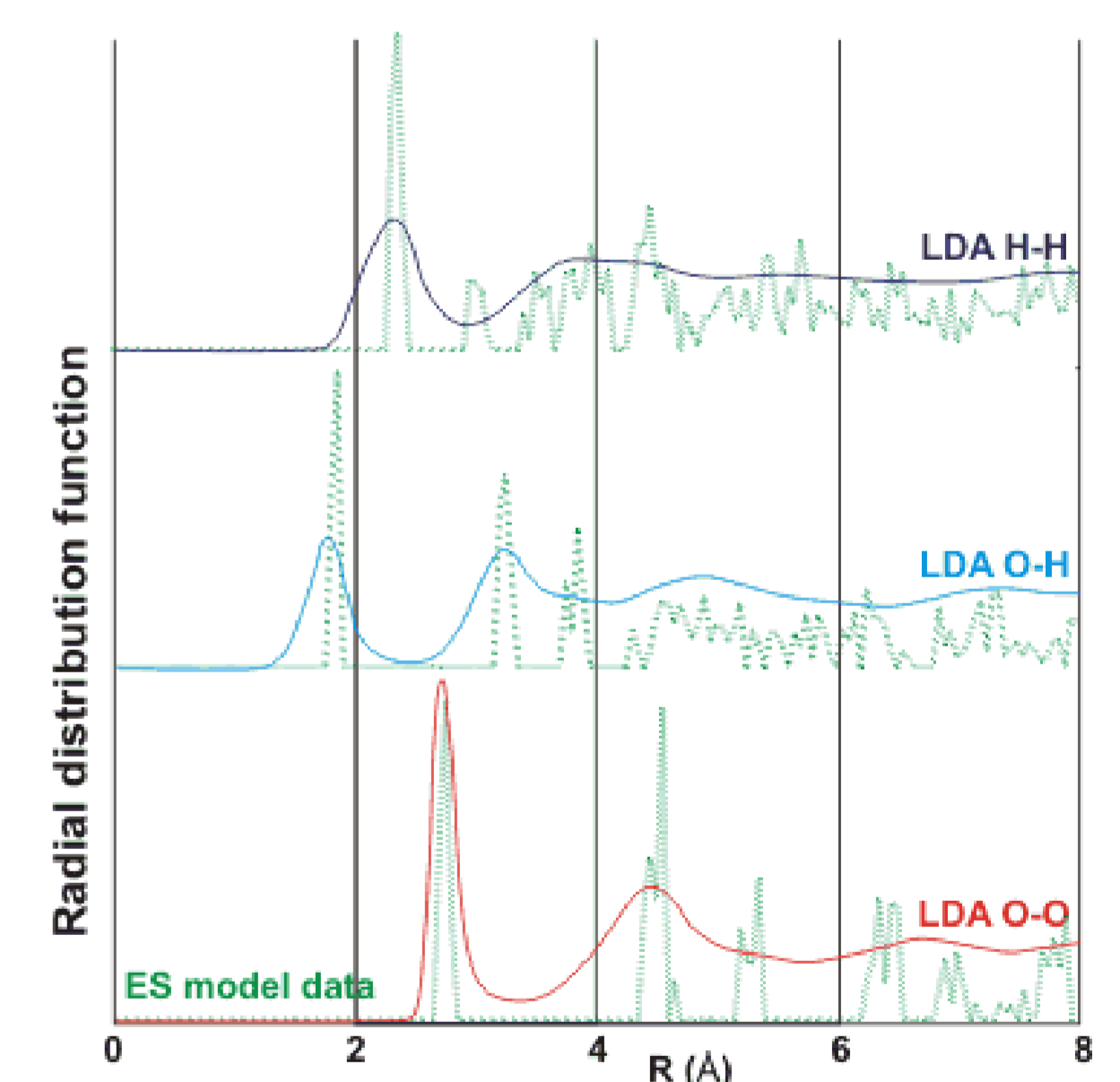
- Chemical inhomogeneity;
- Porosity;
- Processing;
- Instrument accuracy.

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.
- [2] T. D. Bennett, Y. Z. Yue, P. Li, et al., *J. Am. Chem. Soc.*, 2016, **138**, 3484.
- [3] H. Tao, T. D. Bennett and Y. Z. Yue, *Adv. Mater.*, 2017, 1601705
- [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.