



AALBORG UNIVERSITY
DENMARK

Aalborg Universitet

Glass formation mechanism of metal-organic frameworks

Yue, Yuanzheng

Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

[Link to publication from Aalborg University](#)

Citation for published version (APA):
Yue, Y. (2017). Glass formation mechanism of metal-organic frameworks: An invited talk. Abstract from 2017 WPI-AIMR Workshop - Structure and Dynamics of Glasses, Sendai, Japan.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- ? Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- ? You may not further distribute the material or use it for any profit-making activity or commercial gain
- ? You may freely distribute the URL identifying the publication in the public portal ?

Take down policy

If you believe that this document breaches copyright please contact us at vbn@aub.aau.dk providing details, and we will remove access to the work immediately and investigate your claim.

Glass formation mechanism of metal-organic frameworks

Yuanzheng Yue,^{1,2} Ang Qiao,¹ Haizheng Tao,¹ Thomas D. Bennett^{1,3}

¹State Key Laboratory of Silicate Materials for Architectures, Wuhan University of Technology, Wuhan 430070, China.

²Department of Chemistry and Bioscience, Aalborg University, 9220 Aalborg, Denmark.

³Department of Materials Science and Metallurgy, University of Cambridge, Cambridge, CB2 3QZ, United Kingdom

yy@bio.aau.dk

Metal-organic frameworks (MOFs) are microporous inorganic-organic hybrid materials that have been applied in many fields such as gas absorption, catalysis and sensing. In particular, a subset of MOFs called zeolitic imidazolate frameworks (ZIFs) has exhibited a great potential to be used in many areas owing to their tailorable zeolitic structure. Recently, it has been discovered that certain types of ZIFs can melt prior to decomposition, and hence, can be vitrified upon quenching.¹⁻³ However, the mechanism of glass formation of MOFs is a challenging problem to be understood. In this work, we attempt to clarify this problem by characterizing a good MOF glass former, namely, ZIF-62 ($\text{Zn}(\text{Im})_{1.75}(\text{bIm})_{0.25}$). We have found that the ZIF-62 glass is extremely stable against crystallization during heat-treatment. Furthermore, we have observed a pronounced increase of both the glass transition temperature (T_g) and the melting temperature (T_m) of ZIF-62 with increasing the bIm/Im ratio. The T_g/T_m ratio of ZIF-62 is higher than that of any other glass forming systems measured so far, and remains unchanged with the Im/bIm ratio. The viscosity of ZIF-62 at T_m is higher than that of most of the investigated organic and inorganic of glass-forming systems, and but comparable to the fully polymerized strong systems like SiO_2 . By combining these dynamic data with structure analysis, we infer that a balance between the steric hindrance and the degree of the translational motion of structure units is the origin of the high glass forming ability of ZIF-62. The degree of this balance could be the key factor determining whether a MOF can be melted and vitrified.

References:

- 1) T. D. Bennett, J. C. Tan, Y. Z. Yue, E. Baxter, C. Ducati, N. J. Terrill, H. H. M. Yeung, Z. Zhou, W. Chen, S. Henke, A. K. Cheetham, G. N. Greaves, *Nature Commun.* **6** (2015) 8079.
- 2) T. D. Bennett, Y. Z. Yue, P. Li, A. Qiao, H. Z. Tao, G. N. Greaves, T. Richards, G. I. Lampronti, S. A. T. Redfern, F. Blanc, O. K. Farha, J. T. Hupp, A. K. Cheetham and D. A. Keen, *J. Am. Chem. Soc.* **138** (2016) 3484.
- 3) H. Z. Tao, T. D. Bennett, Y. Z. Yue, *Adv. Mater.* **29** (2017) 1601705.