

## Fracture Toughness of a Metal-Organic Framework Glass

Smedskjær, Morten Mattrup; To, Theany; Sørensen, Søren Strandskov; Stepniewska, Malwina; Qiao, Ang; Jensen, Lars Rosgaard; Bauchy, Mathieu; Yue, Yuanzheng

*Publication date:*  
2021

[Link to publication from Aalborg University](#)

### *Citation for published version (APA):*

Smedskjær, M. M., To, T., Sørensen, S. S., Stepniewska, M., Qiao, A., Jensen, L. R., Bauchy, M., & Yue, Y. (2021). *Fracture Toughness of a Metal-Organic Framework Glass*. Abstract from 14th Pacific Rim Conference on Ceramic and Glass Technology, Vancouver, Canada.

### **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](mailto:vbn@aub.aau.dk) providing details, and we will remove access to the work immediately and investigate your claim.

# Fracture Toughness of a Metal-Organic Framework Glass

Theany To<sup>1</sup>, Søren S. Sørensen<sup>1</sup>, Malwina Stepniewska<sup>1</sup>, Ang Qiao<sup>1</sup>, Lars R. Jensen<sup>2</sup>, Mathieu Bauchy<sup>3</sup>,

Yuanzheng Yue<sup>1</sup>, Morten M. Smedskjaer<sup>1</sup>

<sup>1</sup> *Department of Chemistry and Bioscience, Aalborg University, Aalborg, Denmark*

<sup>2</sup> *Department of Materials and Production, Aalborg University, Aalborg, Denmark*

<sup>3</sup> *Department of Civil and Environmental Engineering, University of California, Los Angeles, USA*

## Abstract

Metal-organic framework (MOF) glasses feature unique thermal, structural, and chemical properties compared to traditional metallic, organic, and oxide glasses. In practical engineering, the knowledge of their strength and toughness are important, yet the small sizes of MOF glasses limits the testing. Recently, the discovery of a zeolitic imidazolate framework (ZIF) glass with ultra-high glass forming ability, namely ZIF-62, has enabled the preparation of >25 mm<sup>3</sup> samples and thus mechanical testing besides indentation. In this work, we report the first measurement of the fracture toughness ( $K_{Ic}$ ) of a bulk MOF material using a self-consistent single-edge precracked beam method and find it to be  $\sim 0.1 \text{ MPa m}^{0.5}$ , which is low even compared to brittle oxide glasses and in between the values of foam and elastomers. Molecular dynamics simulations and theoretical calculations confirm the low  $K_{Ic}$  value of ZIF-62 glass, ascribing the origin to the weak coordinative bonds (Zn-N), which preferentially break during crack propagation.

## References:

To T., Sørensen S. S., Stepniewska M., Qiao A., Jensen L. R., Bauchy M., Yue Y. Z., Smedskjaer M. M. Fracture Toughness of a Metal-Organic Framework Glass. *Nature Communications* **11**, 2593 (2020).

To T., Sørensen S. S., Yue Y. Z., Smedskjaer M. M. Bond switching is responsible for nanoductility in zeolitic imidazolate framework glasses. *Dalton Transactions* **50**, 6126-6132 (2021).