



AALBORG UNIVERSITY
DENMARK

Aalborg Universitet

Thermal Conductivity of Zeolitic Imidazolate Framework Glasses

Sørensen, Søren Strandskov; Østergaard, Martin Bonderup; Stepniewska, Malwina; Johra, Hicham; Yue, Yuanzheng; Smedskjær, Morten Mattrup

Publication date:
2021

[Link to publication from Aalborg University](#)

Citation for published version (APA):

Sørensen, S. S., Østergaard, M. B., Stepniewska, M., Johra, H., Yue, Y., & Smedskjær, M. M. (2021). *Thermal Conductivity of Zeolitic Imidazolate Framework Glasses*. Poster presented at 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 providing details, and we will remove access to the work immediately and investigate your claim.

Thermal Conductivity of Zeolitic Imidazolate Framework Glasses

Søren S. Sørensen¹, Martin B. Østergaard¹, Malwina Stepniewska¹, Hicham Johra², Yuanzheng Yue¹, Morten M. Smedskjaer¹

¹ *Department of Chemistry and Bioscience, Aalborg University, Denmark*

² *Department of the Built Environment, Aalborg University, Denmark*

Generally, crystals are known to have higher thermal conductivity than their isochemical glasses due to stronger phonon scattering in the latter. In this work, we report the inverse relation for a recently discovered family of zeolitic imidazolate framework (ZIF) glasses by both experiments and reactive molecular dynamics (MD) simulations. That is, we find that the studied ZIF-4 and ZIF-62 glasses possess *higher* thermal conductivity than their isochemical crystals. We ascribe the effect to the anomalous density increase of the ZIF systems upon vitrification combined with the strong phonon scattering in the crystalline ZIFs. The effect is further verified by simulating a ZIF-8 glass and its corresponding and highly porous crystal. Finally, we probe the phonon characteristics by MD simulations, showing that the low-frequency modes are the main contributors to heat conduction.

Reference: Sørensen S. S., Stepniewska M., Østergaard M. B., Johra H., Yue Y. Z., Smedskjaer M. M. Metal-Organic Framework Glasses Possess Higher Thermal Conductivity than Their Crystalline Counterparts. *ACS Applied Materials & Interfaces* **12**, 18893-18903 (2020).