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

Thermal Conductivity of Zeolitic Imidazolate Framework Glasses

Søren S. Sørensen[1], Martin B. Østergaard[1], Malwina Stepniewska[1], Hicham Johra[2], Yuanzheng Yue[1], Morten M. Smedskjaer[1]

[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).