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*Publication date:*
2021

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## 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 $mm^3$ 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 ~0.1 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).