# Fracture Toughness of Zeolitic Imidazolate Framework Glasses

*Invited Talk*

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## Fracture toughness of zeolitic imidazolate framework glasses

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Metal-organic frameworks (MOFs) are a class of organic-inorganic hybrid materials with high porosity. Recently, it has been discovered that a subset of MOFs, namely zeolitic imidazolate frameworks (ZIFs), can be melted and quenched into glasses. This makes it possible to prepare bulk, transparent ZIF glasses with modifiable organic and inorganic building units. To enable their applications, there is a need to understand the mechanical properties. In this work, we study the fracture toughness ($K_{Ic}$) of ZIF glasses using both experiments and reactive molecular dynamics simulations. Although the glasses exhibit pronounced ductility at the nanoscale, we find that $K_{Ic}$ is on the order of 0.1 MPa $m^{0.5}$, which is even lower than that of brittle oxide glasses. We ascribe these phenomena to the preferential breakage and switching of the weak coordination Zn-N bonds. The observed Zn-N bond switching mechanism is found to be more pronounced for smaller organic linkers.

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