Electronic Supplementary Information

Bond switching is responsible for nanoductility in zeolitic imidazolate framework glasses

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Supplementary Tables

Table S1: Average number of broken bonds, for which either N or Zn is a part of the bond, relative to the total number of broken bonds at the point of maximum strain for each glass type. It can be observed that bonds connecting N and Zn are nearly exclusively broken during the fracture process.

	Broken N-related bonds relative to total number of broken bonds (%)	**Broken Zn-related bonds relative to total number of broken bonds (%)**
ZIF-4	99.6	98.6
ZIF-62	99.7	99.5
ZIF-76	99.5	98.8

Supplementary Figures

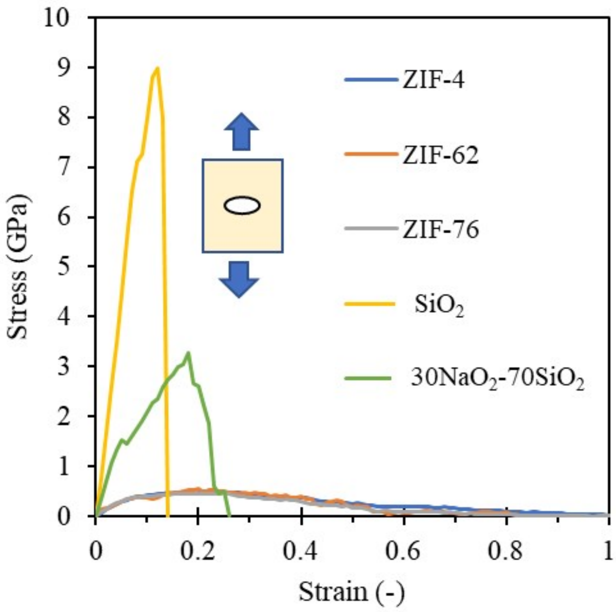
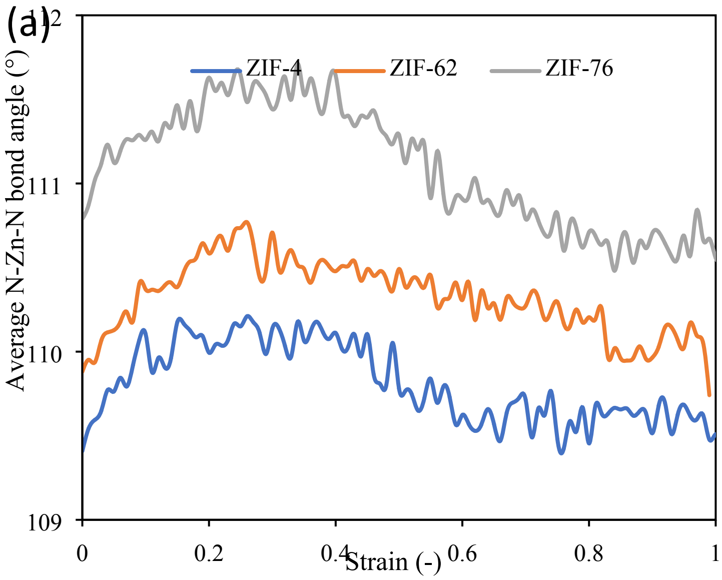


Figure S1: Stress-strain curves of simulated SiO_2 (yellow) and $30Na_2O$-$70SiO_2$ (green) glasses from ref.[7], as well as the ZIF-4, ZIF-62, and ZIF-76 glasses from this study and ref.[1], highlighting the pronounced nanoductility of the ZIF glasses.



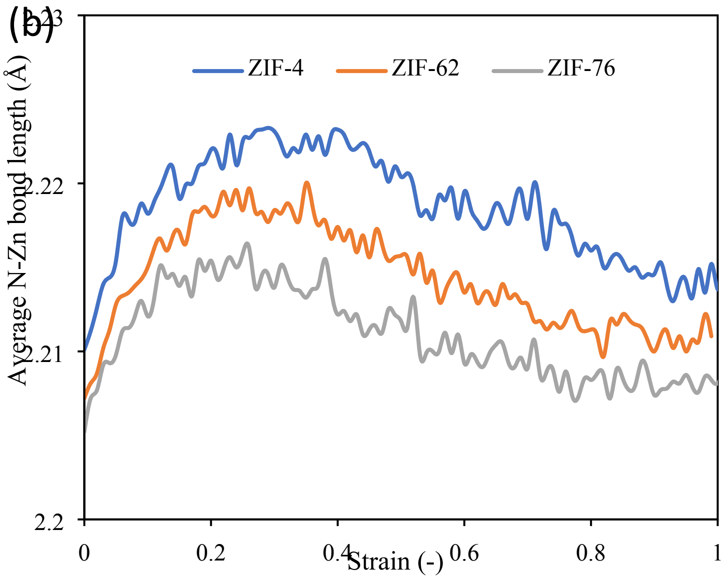


Figure S2: (a) Average N-Zn-N bond angle and (b) average N-Zn bond length of the three ZIF glasses during applied tensile strain in MD simulations from 0 to 100% strain.

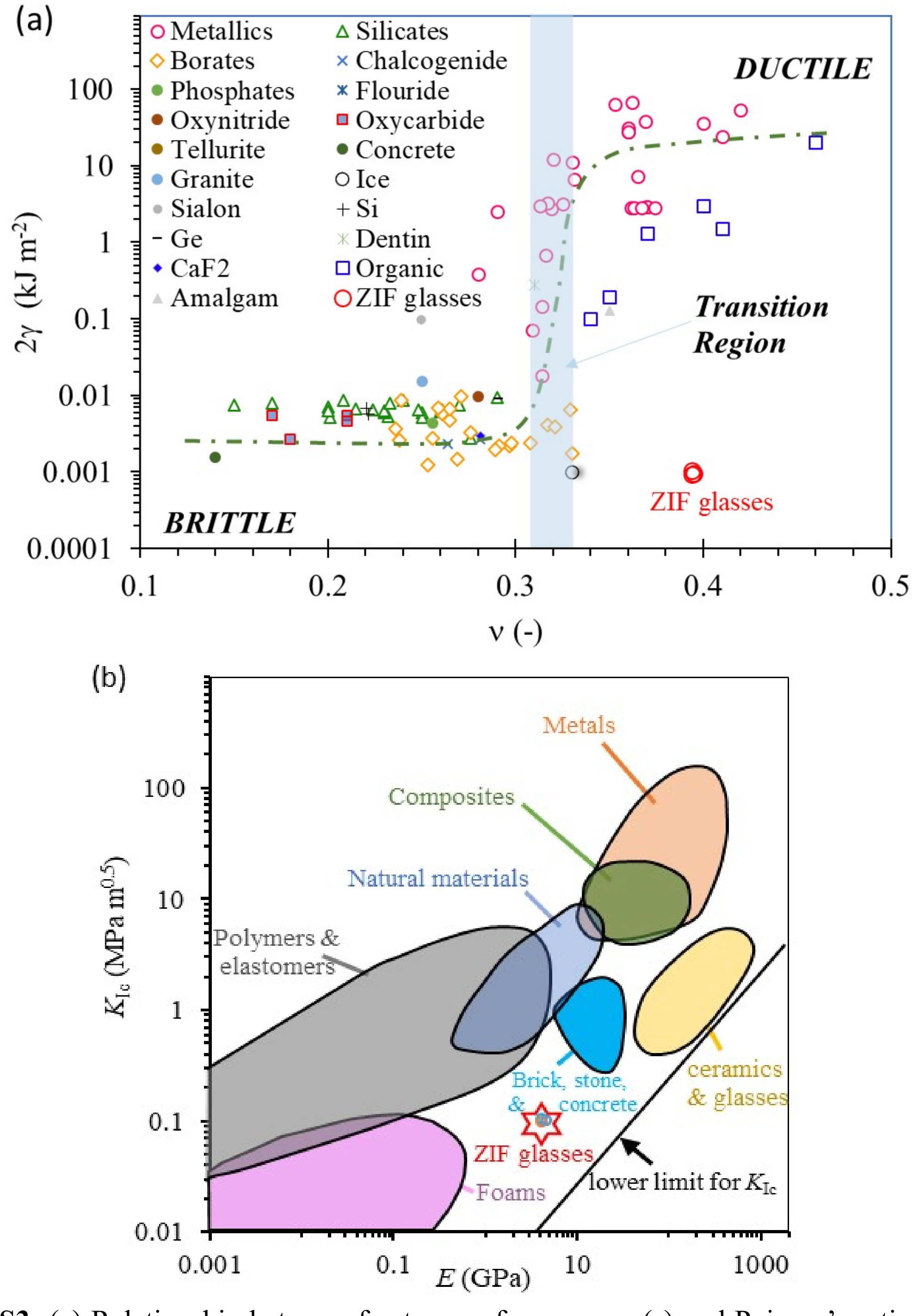


Figure S3: (a) Relationship between fracture surface energy (*γ*) and Poisson's ratio (*v*) for a range of materials. The figure is adopted from Ref.[1], but extended with the data from Refs.[11–13] and additional data for metallic glasses[14–17], silicate glasses[18–20], borate glasses[20–23], chalcogenide glasses[22,24,25], phosphate glasses[22,26], fluoride glasses[19,22], oxycarbide glasses and glass ceramics[10,20], tellurite glass[22], and the present ZIF glasses. (b) Relation between fracture toughness and Young's modulus for a range of materials. The figure is adopted with the data from the Ashby plot[17] and extended with those of the present ZIF glasses.

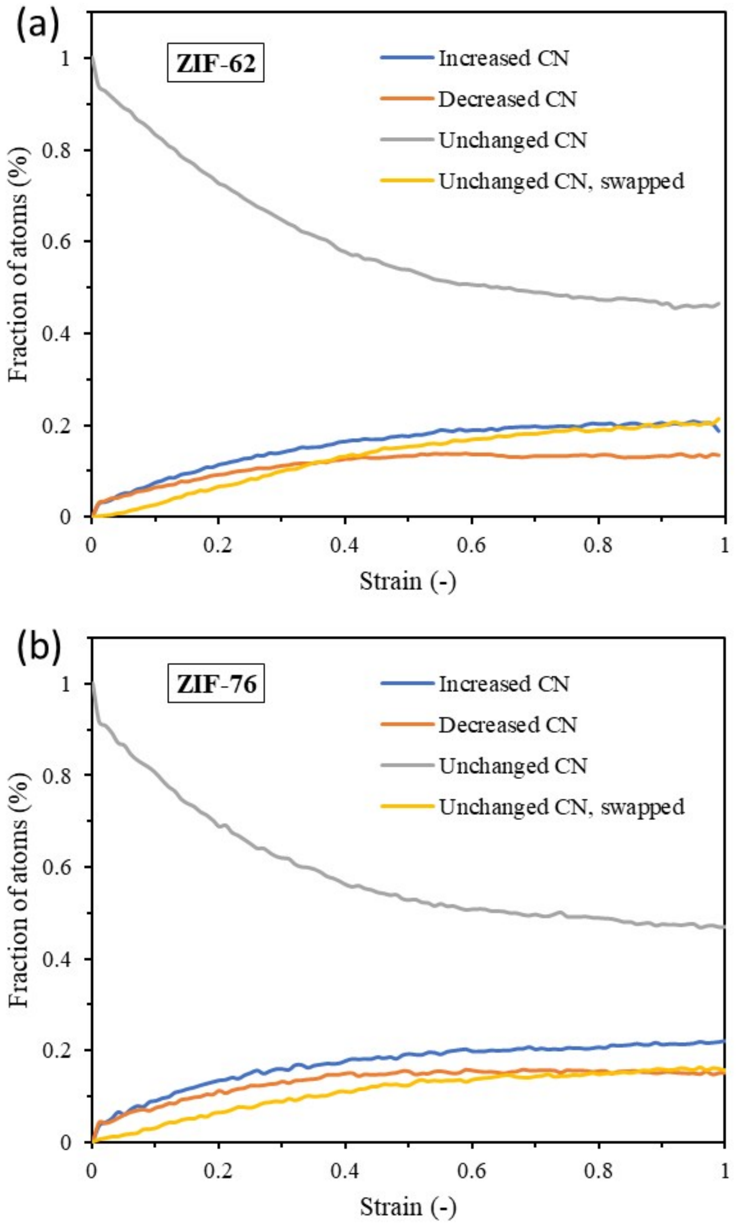


Figure S4: Average changes in Zn-N bonding during applied tensile strain in MD simulations from 0 to 100 % strain for (a) ZIF-62 glass and (b) ZIF-76 glass.

Supplementary References

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