Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Thermodynamic features and enthalpy relaxation in a metal-organic framework glass

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ESI: Figures S1-S4.

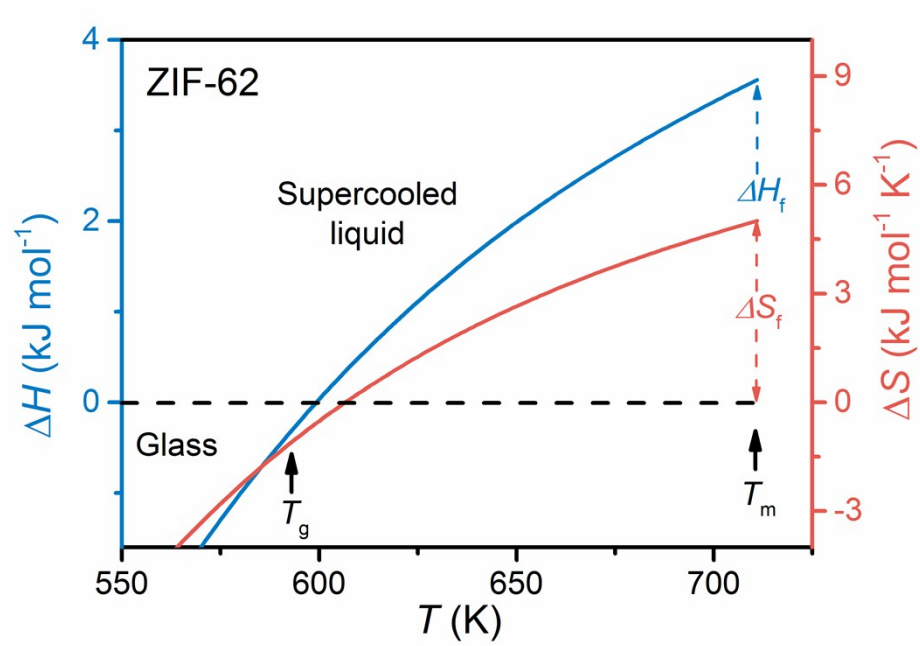

Fig. S1 Differences in enthalpy $\Delta H^{sl-x}(T)$ and entropy $\Delta S^{sl-x}(T)$ between the supercooled liquid and crystal in ZIF-62.

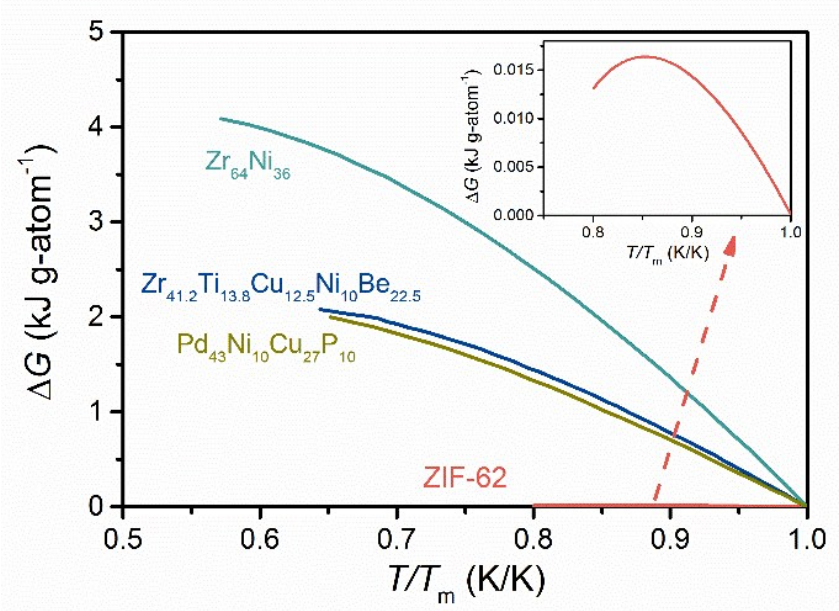

Fig. S2 Differences in the Gibbs free energy difference $\Delta G^{sl-x}(T)$ between the supercooled liquid and the crystal of ZIF-62, using a kJ g-atom^{-1} basis (18.5 atoms per ZIF-62 molecule according to the formula). The $\Delta G^{sl-x}(T)$ of some alloys are also given as comparisons from literature, in which one atom is taken as per mol.

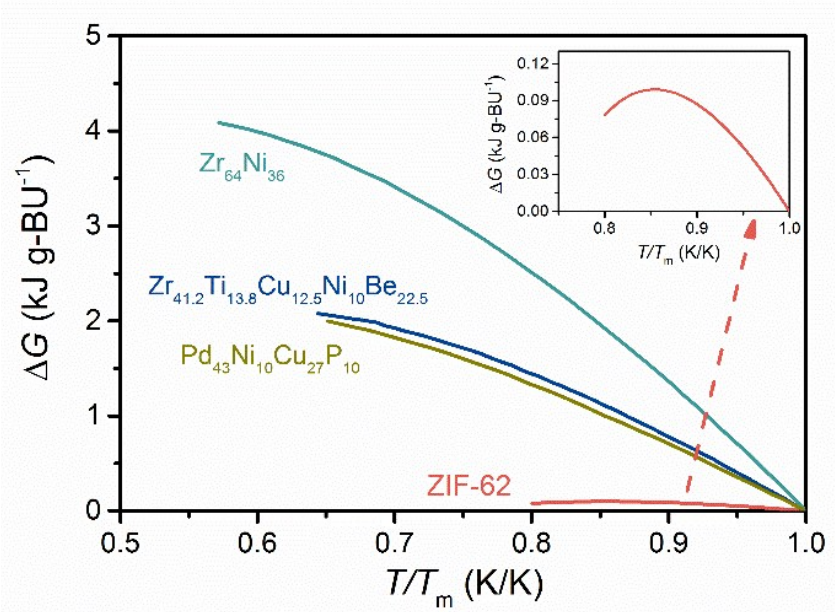

Fig. S3 Differences in the Gibbs free energy difference $\Delta G^{sl-x}(T)$ between the supercooled liquid and the crystal of ZIF-62, using a kJ g-BU^{-1} basis (BU: building unit, referring to Imidazolate, benzimidazolate and Zn^{2+}. Each ZIF-62 $[Zn(Im)_{1.75}(bIm)_{0.25}]$ molecule has three BUs.) The $\Delta G^{sl-x}(T)$ of some alloys are also given as comparisons from literature, in which one BU is taken as per mol.

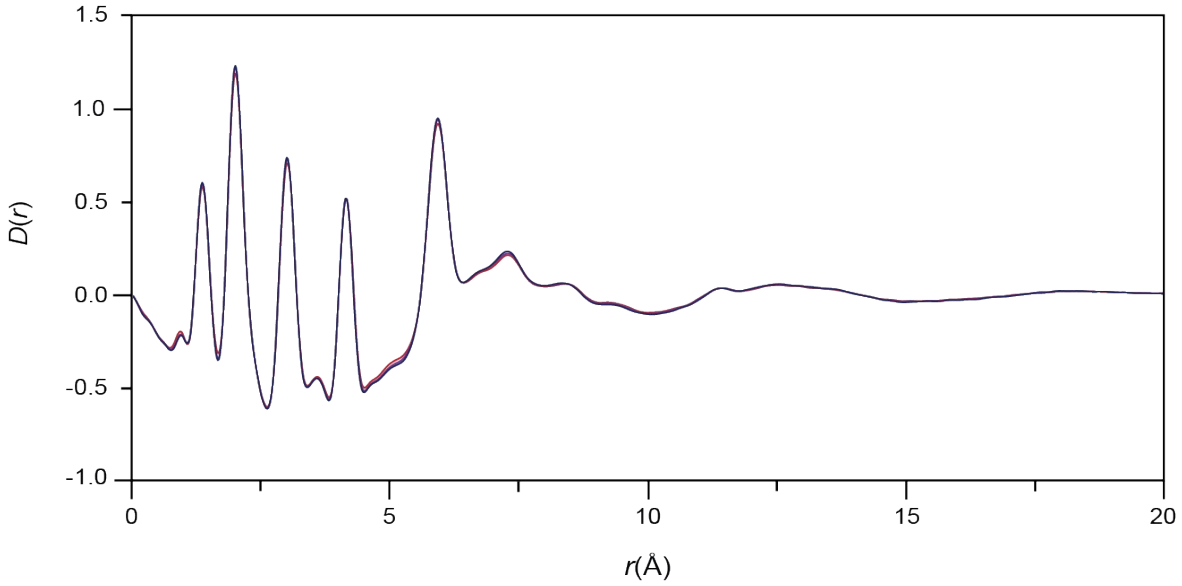

Fig. S4 Pair distribution function, D(r) of a_gZIF-62 after melt quenching (red), annealed at 553 K with no duration (t_a=0) (purple), and annealed at 553 K for 72 hours (blue) in the region of 0~20 Å.