

Supplementary information for:

**Structure of Metal–Organic Framework Glasses
by Ab Initio Molecular Dynamics**

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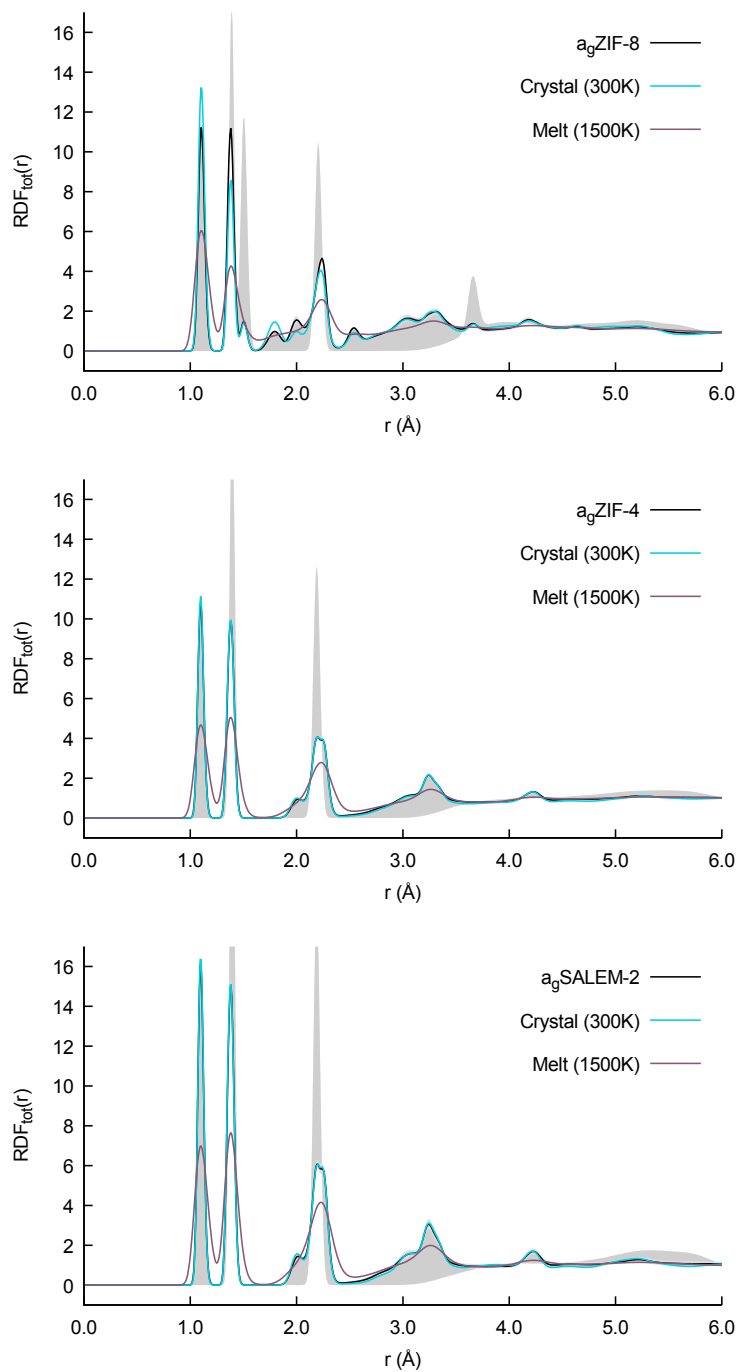


Figure S1. Total radial distribution functions (RDF) for the three structures. In light blue we remind the crystalline RDF obtained from previous simulations, in purple we plot the average RDF for the melt at 1,500 K and in black the average RDF over all the glass configurations. To give an idea of the variance exhibited by the ten different trajectories, the filled curves in light gray correspond to the black curve plus or minus the standard deviation associated with the ten samples.

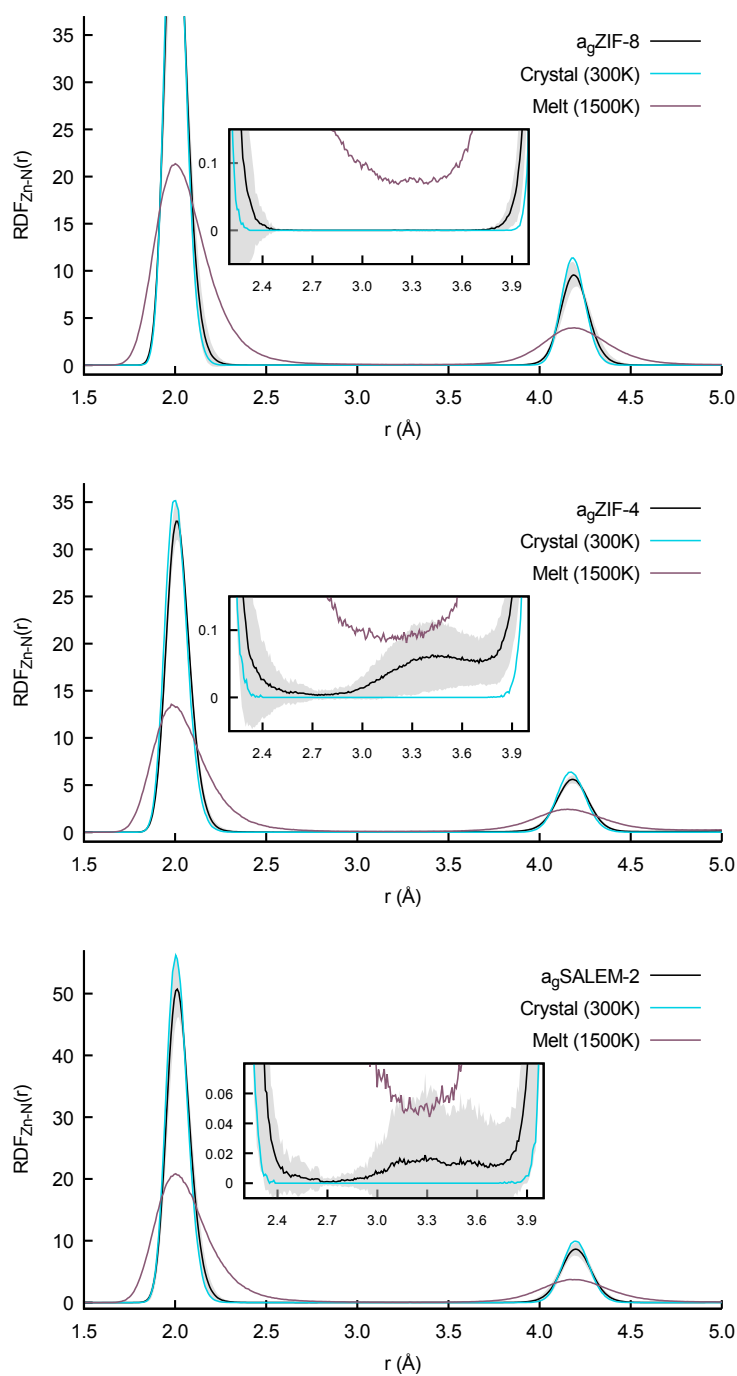


Figure S2. Radial distribution functions (RDF) for the Zn–N pair for the three structures. In light blue the crystalline RDF obtained from previous simulations is shown, in purple the average RDF for the melt at 1,500 K and in black the average RDF over all the glass configurations. The light gray areas correspond to the standard deviation between the ten trajectories. Cumulative functions corresponding to the number of neighbors are shown (in green for the glass, in blue for the crystal). The inset in each graph show a zoom on the region between 2.2 and 4.0 Å.

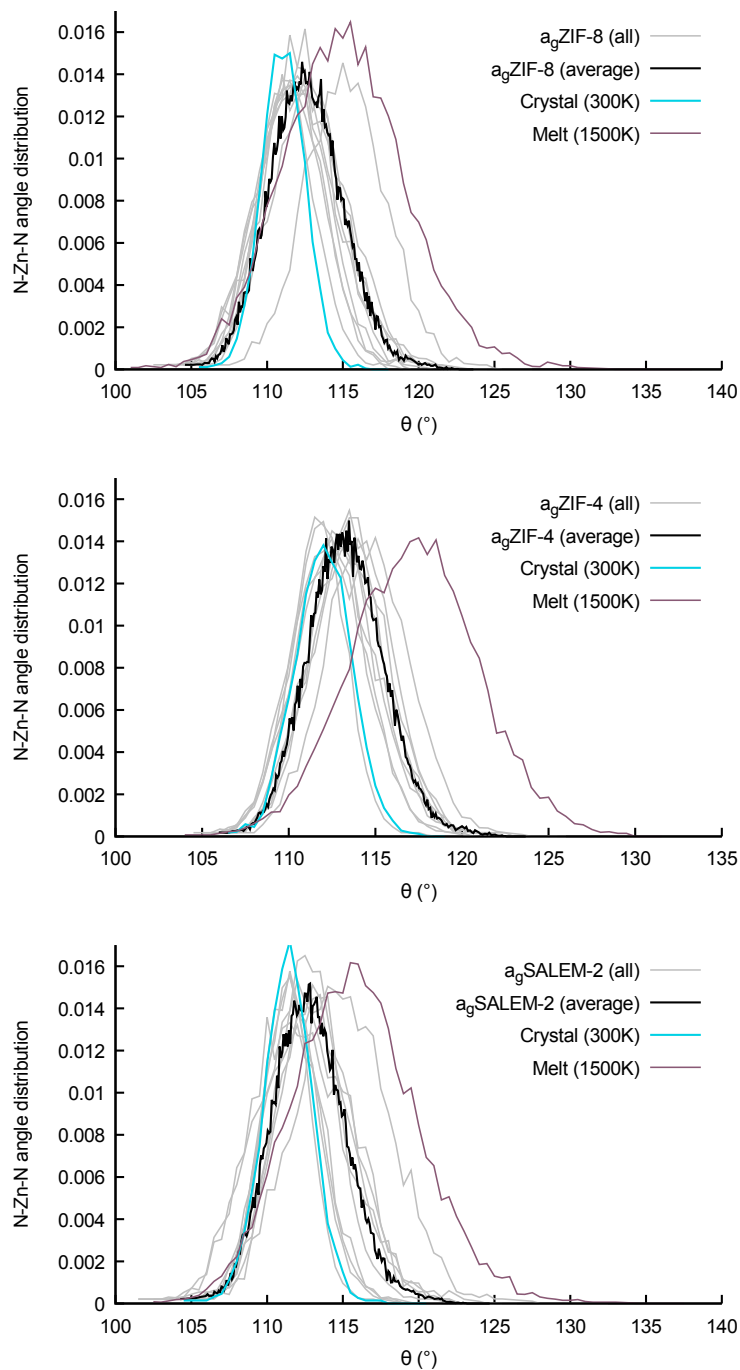


Figure S3. Distributions of the N–Zn–N angle for the three frameworks in the three phases (crystalline (light blue), molten (purple) and glass (black)). The light gray curves correspond to the ten different initial configurations for each framework.

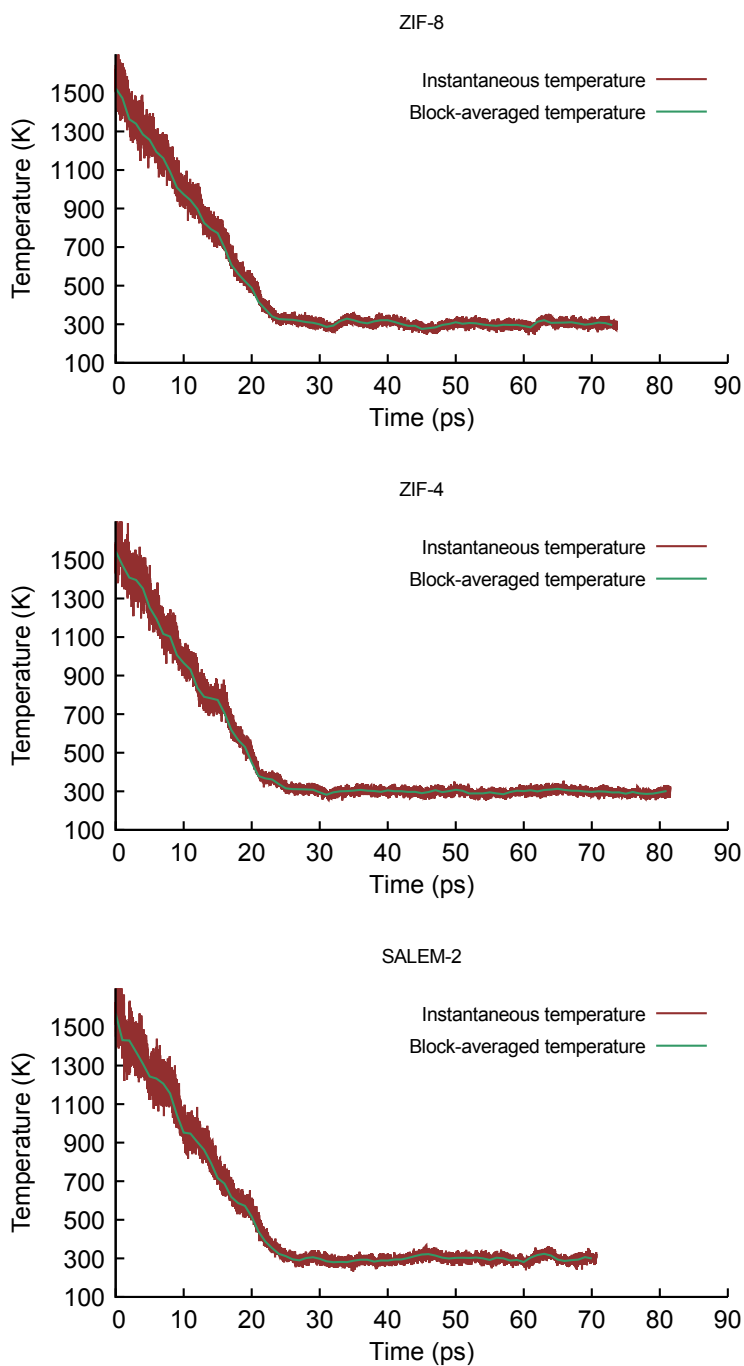


Figure S4. Examples of the instantaneous temperatures resulting from the imposed decrease of temperature. The instantaneous temperature is shown in red and its block-averaged value (per block of 1 ps) is shown in green.