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

Structural origin of high glass-forming ability of Ce70Ga10Cu20 alloy

To further illustrate the short-range orders around Ga and Cu atoms, atomic collective alignment method is employed to show the average coordination environment in the melts [1, 2]. The obtained atomic density distributions around Ga and Cu atoms in the $Ce_{70}Ga_xCu_{30-x}$ (x = 6, 10 and 13) melts are shown in Figure S1. From the figure, one can see that Ga-centered clusters exhibit a strong icosahedral short-range order (ISRO) in $Ce_{70}Ga_xCu_{30-x}$ (x = 6, 10 and 13) melts，which is agree with Voronoi tessellation analysis. The average coordination environment of Cu is also shown in Figure S1. One can see that the number of the separated regions around Cu decreases with the concentration of Ga, which is agree with the variation of the coordination number of Cu. Furthermore, five-fold symmetry around Cu atoms are observed for all the compositions. As is known, fivefold symmetry is not compatible with the crystal symmetry and thus the short-range order benefits the glass formation ability.

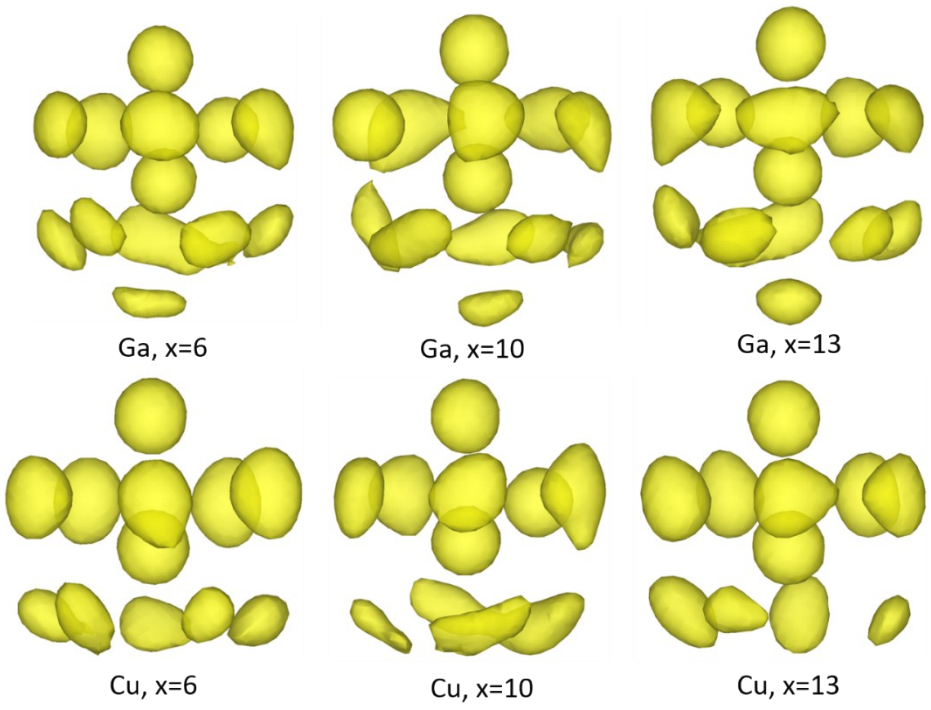

Figure S1 Atomic-density contour plot of the final configuration of the atomic collective alignment around Ga and Cu in $Ce_{70}Ga_xCu_{30-x}$ (x= 6, 10 and 13) melts.

1 X. W. Fang, C. Z. Wang, Y. X. Yao, Z. J. Ding, and K. M. Ho, Phys. Rev. B 82, 184204 (2010).

2 X. W. Fang, C. Z. Wang, Y. X. Yao, Z. J. Ding, and K. M. Ho, Phys. Rev. B 83, 224203 (2011).