Electronic Supplementary Material (ESI) for Nanoscale.

Tempering of Au nanoclusters: capturing the temperature-dependent competition among structural motifs

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Electronic Supplementary Information

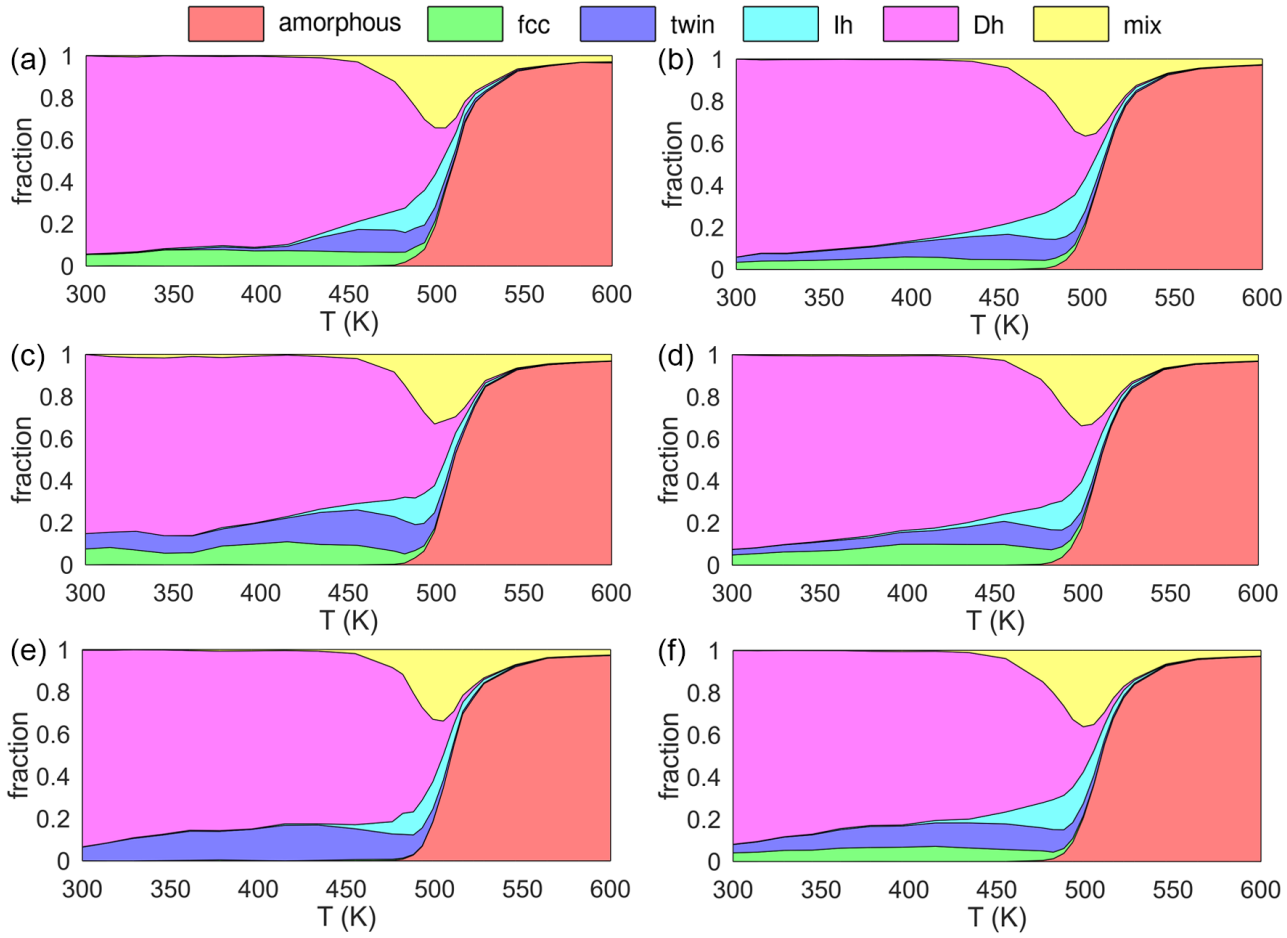

Fig. S 1. PTMD simulations of Au_{147} nanoclusters. Fraction of structures as a function of temperature for initial structure Dh (global minimum) at (a) 0.5 μs and (b) 2.4 μs. Fraction of structures as a function of temperature for initial structure twin at (c) 0.5 μs and (d) 2.4 μs. Fraction of structures as a function of temperature for initial structure random at (e) 0.6 μs and (f) 2.4 μs.

In the Fig. S1, we compare the results of PTMD simulations for three different initial structures: Dh (a,b), twin (c,d), and non-physical random (e,f). After a time of about 0.5 μs to 0.6 μs, there are differences between the three PTMD simulations. However, after 2.4 μs, all the three simulation converge to the same structural distribution.