

Supporting Information

Investigation of thermal properties of phase change materials encapsulated into capped carbon nanotubes using molecular dynamics simulations

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Table S1. The different QSC interaction parameters used in this work.^{46,47}

Interaction	ε (eV)	a (Å)	n	m	c
Cu-Cu	0.0057921	3.6030	10	5	84.843
Ag-Ag	0.0039450	4.0691	11	6	96.524
Al-Al	0.0014253	4.0500	7	6	16.399

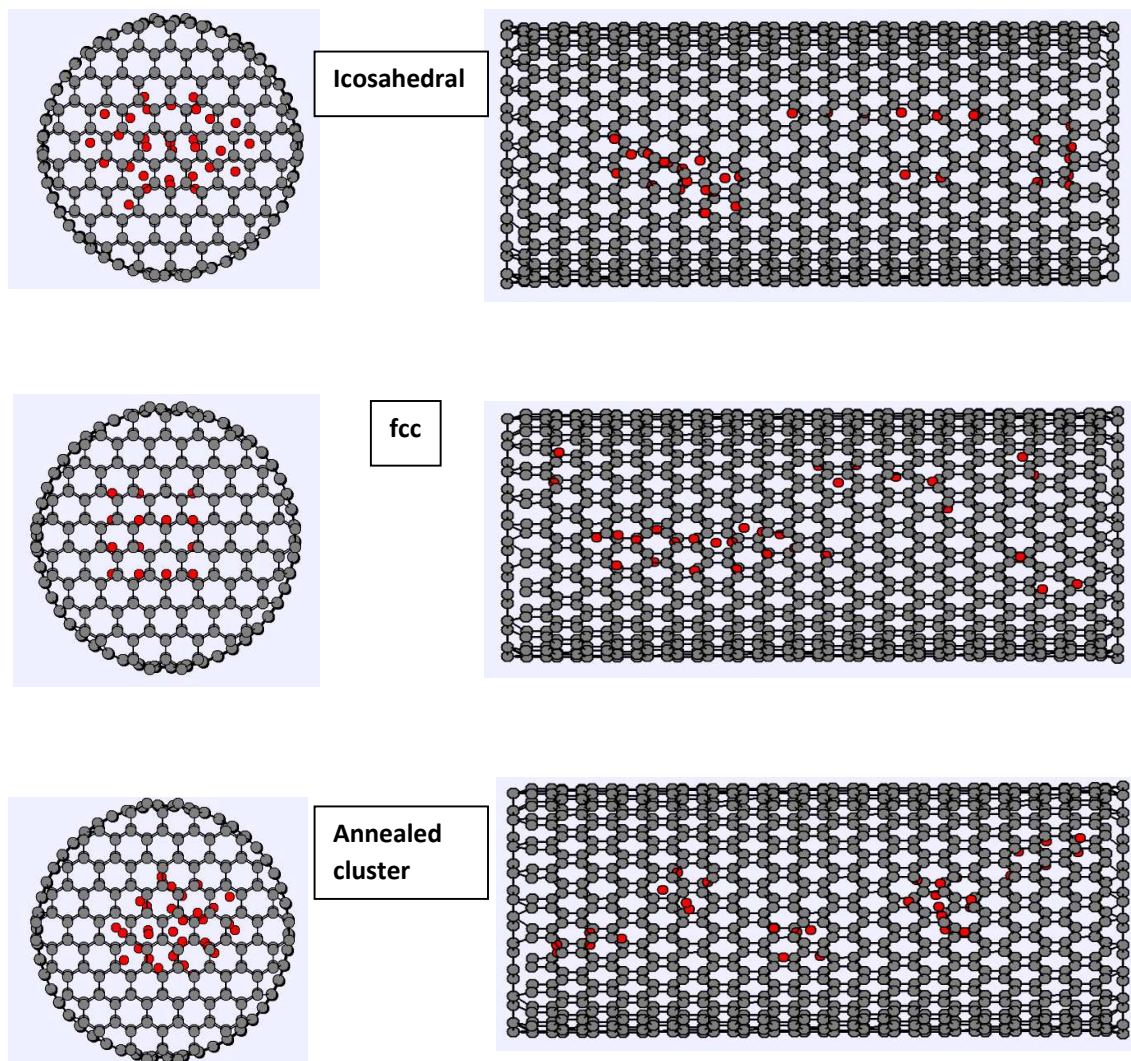


Fig. S1. The snapshots of the test simulation results for the Ag nanocluster system with the different initial structures for the silver nanocluster at the initials and after 0.7 ns of the simulation times.

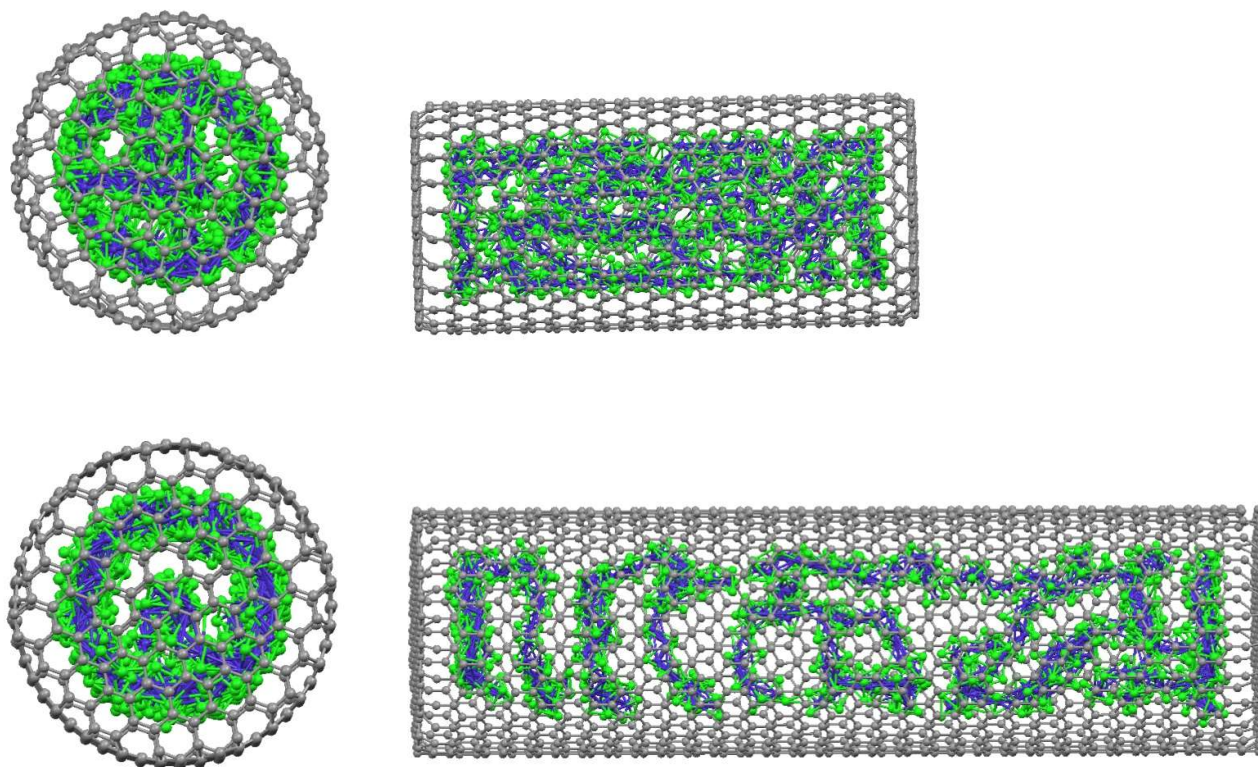


Fig. S2. The snapshots of the octadecane molecules into both normal and long CNTs at the same temperature ($T=305$ K). The carbon atoms of CNTs are in gray, the carbon atoms of alkanes are in blue, and the hydrogen atoms are in green.

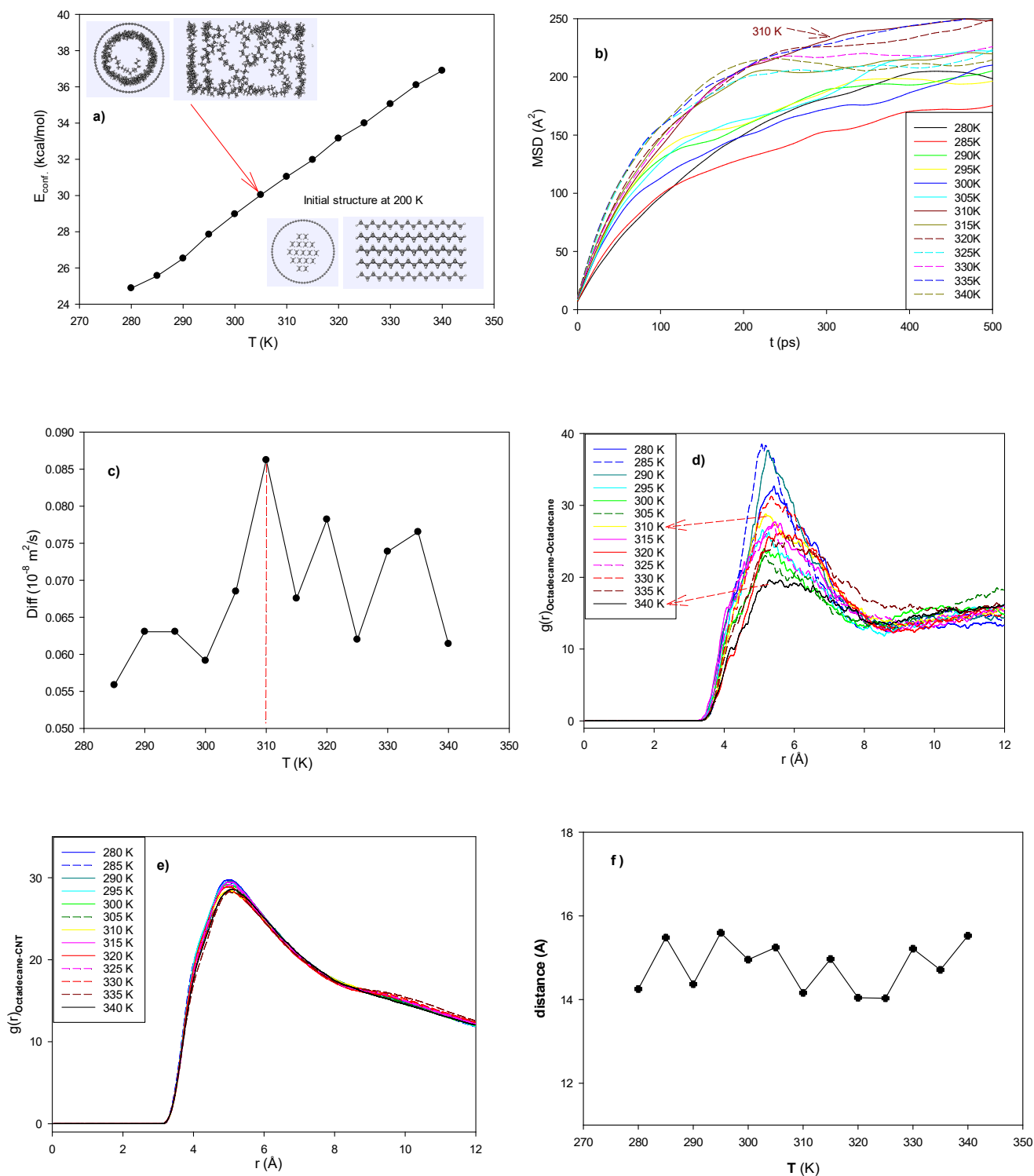


Fig. S3. The CNT diameter effect; a) configurational energy, b) MSD, c) self-diffusion coefficient, d) octadecane-octadecane RDF, e) octadecane-CNT RDF, and f) average end-to-end distance of the confined molecules into capped (30,0) CNT. The standard errors of the energy and diffusion points are as the same order of the normal system (Fig. 1).

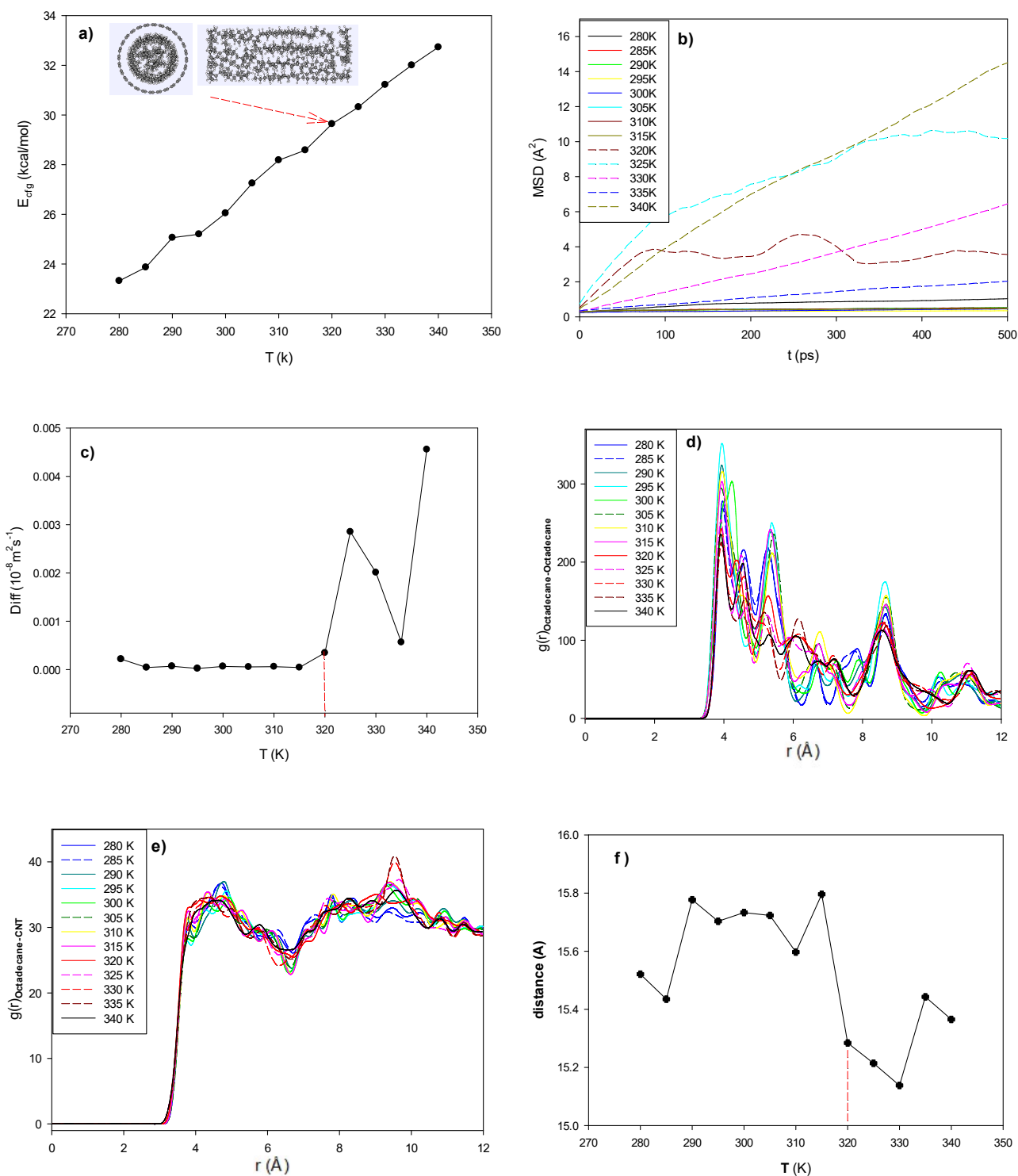


Fig. S4. The CNT chirality effect; a) configurational energy, b) MSD, c) self-diffusion coefficient, d) octadecane-octadecane RDF, e) octadecane-CNT RDF, and f) average end-to-end distance of the confined molecules into capped (14,14) CNT. The standard errors of the energy and diffusion points are as the same order of normal system (Fig. 1).

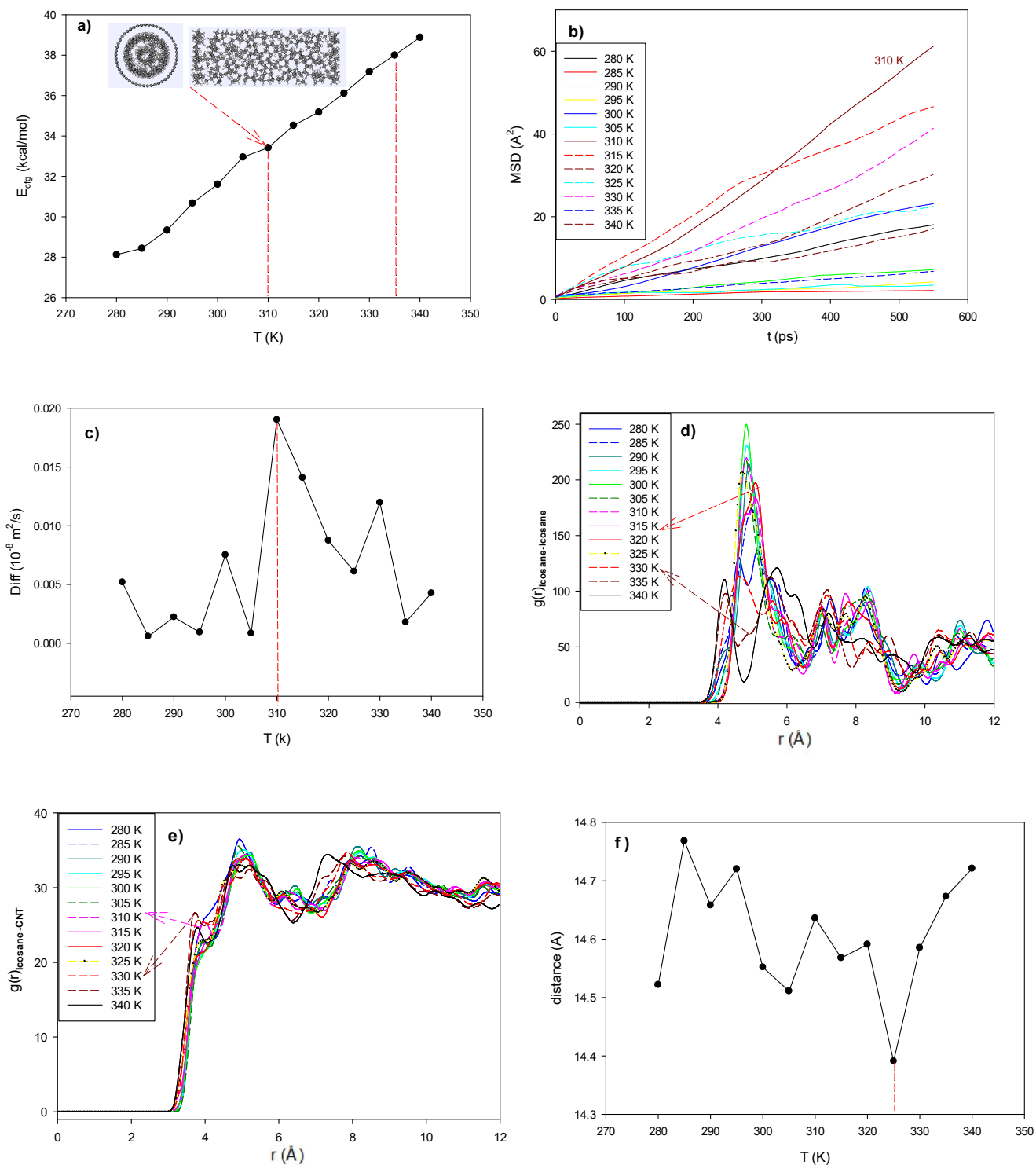


Fig. S5. The effect of alkane chain; a) configurational energy, b) MSD, c) self-diffusion coefficient, d) icosane-icosane RDF, e) icosane-CNT RDF, and f) average end-to-end distance of the confined molecules into capped (25,0) CNT. The standard errors of the energy and diffusion points are as the same order of normal system (Fig. 1).

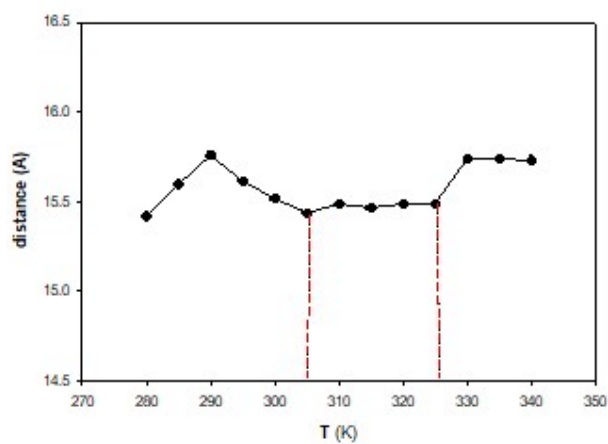
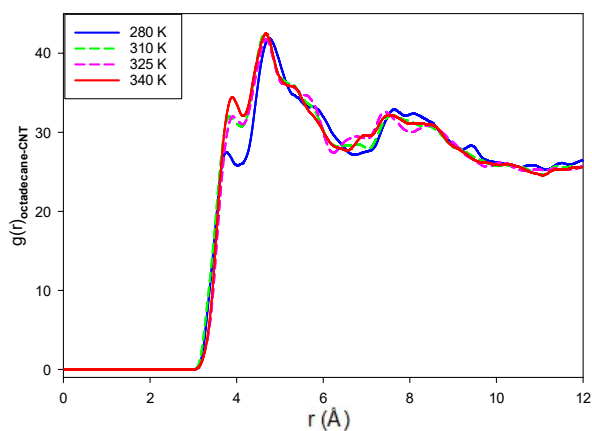
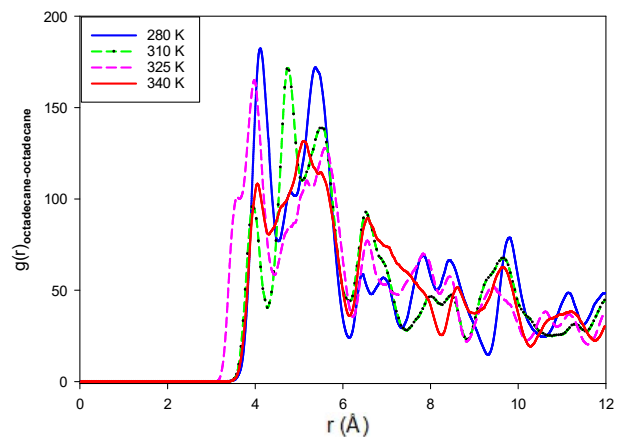
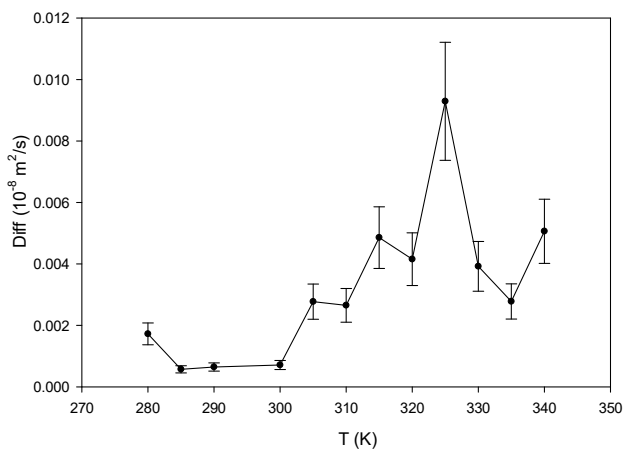
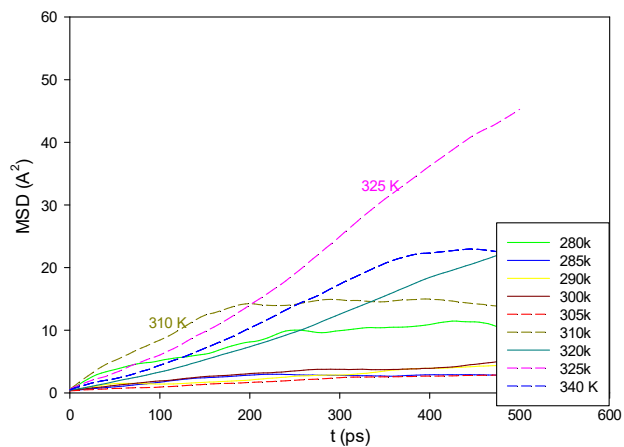
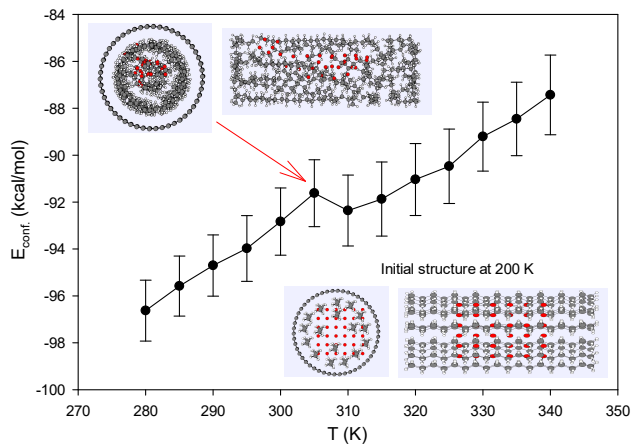


Fig. S6. The Ag cluster system; a) configurational energy, b) MSD, c) self-diffusion coefficient, d) octadecane-octadecane RDF, e) octadecane-CNT RDF, and f) average end to end distance.

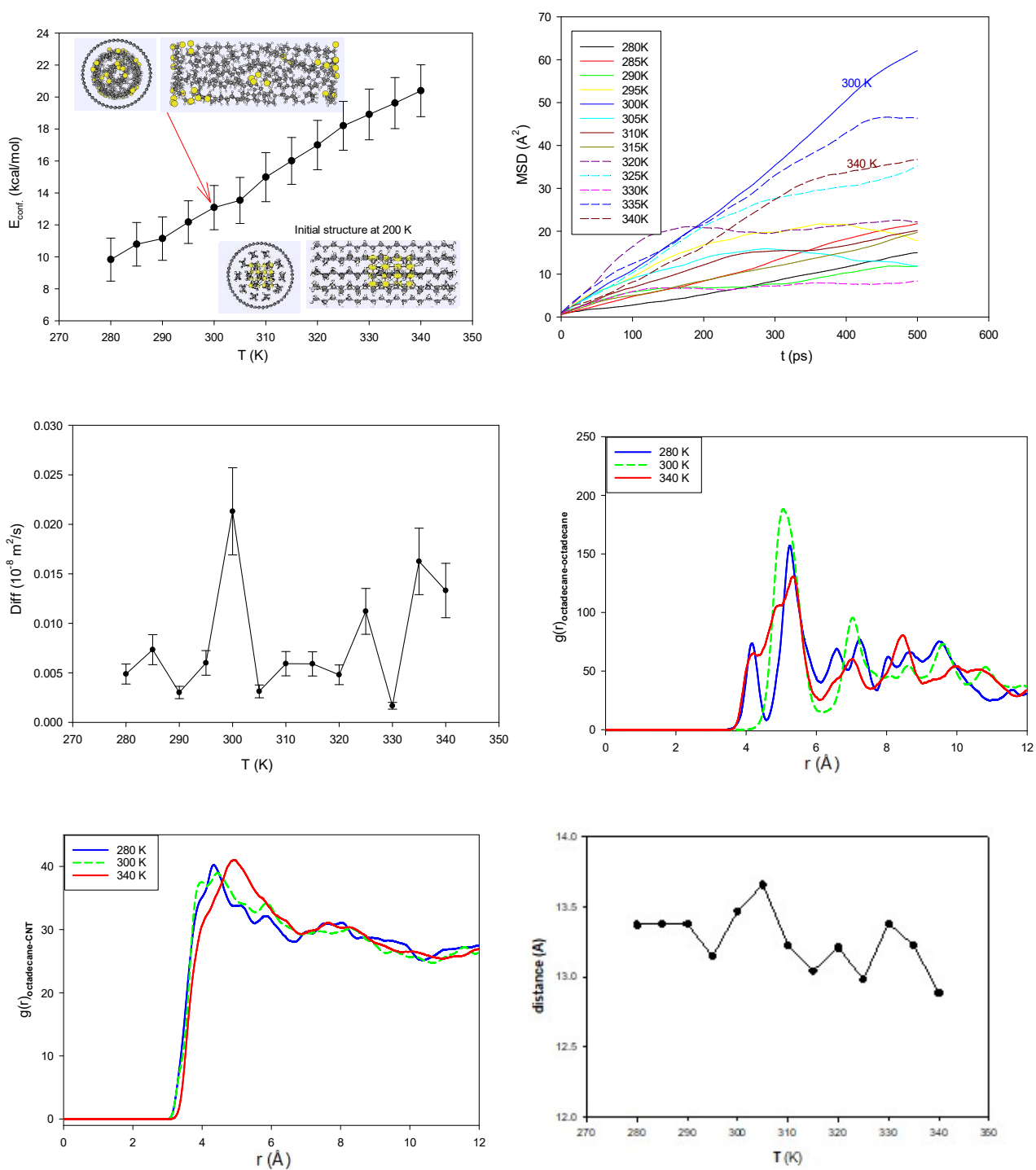


Fig. S7. The Al cluster system; a) configurational energy, b) MSD, c) self-diffusion coefficient, d) octadecane-octadecane RDF, e) octadecane-CNT RDF, and f) average end to end distance.

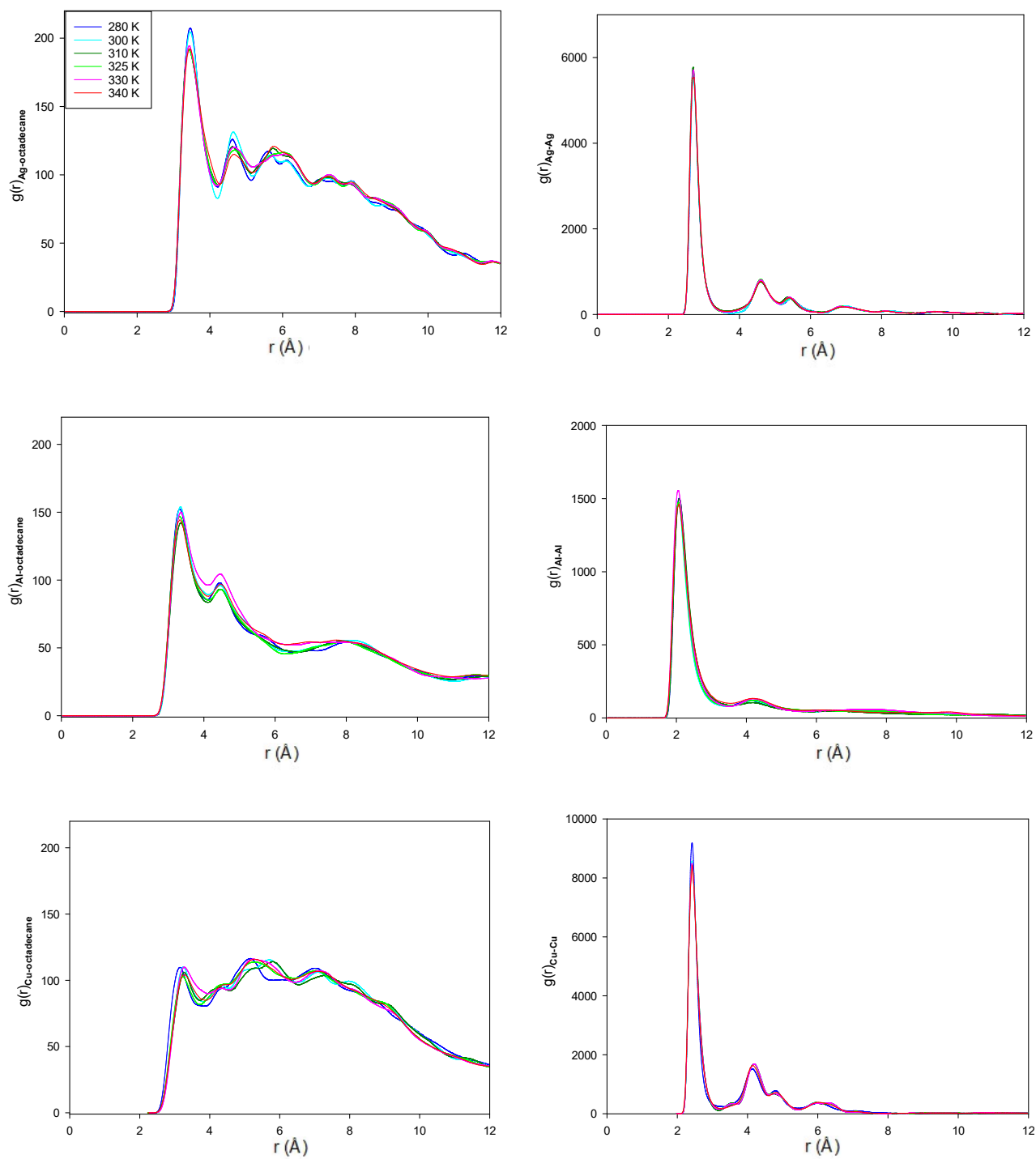


Fig. S8. The cluster-octadecane and cluster-cluster RDFs in the different systems at the different temperatures.