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The Initial Stages of Melting of Graphene Studied Between 4000 K and 6000 K

Supplemental Information

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The CASTEP computational parameters were: Accuracy = fine; Self-Consistent Field (SCF) = 1×10^{-6}; Smearing = 0.06; history length of 20; Nosé–Hoover method, Nosé Q = 2, Nosé chain length = 2; cutoff energy = 400 eV; Fixed center of mass. The DFT method was DFT-D GGA, PBE.

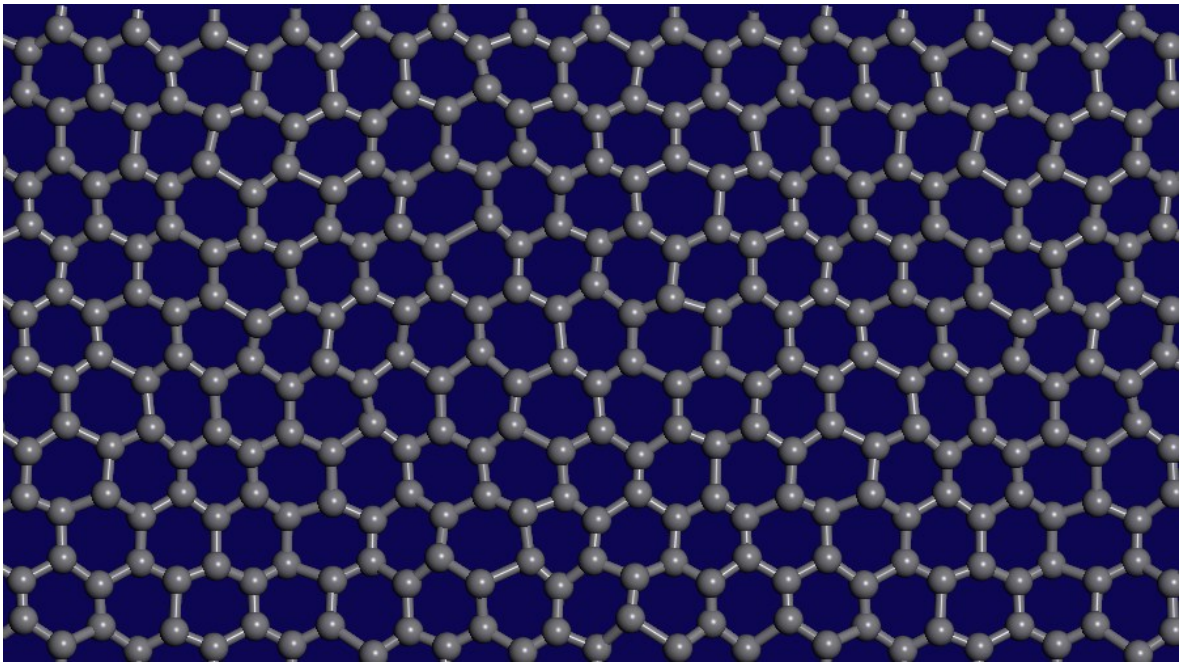

Figure S1. Last frame of the 4000 K simulation, top view.

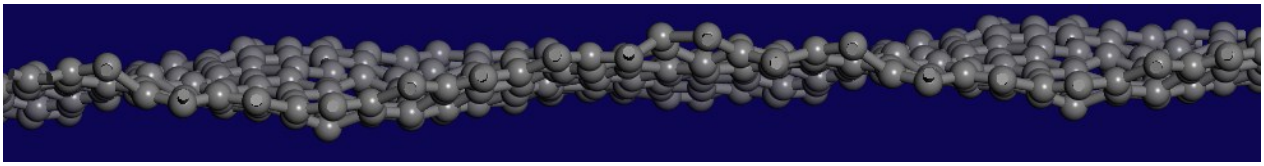

Figure S2. Last frame of the 4000 K simulation, side view.

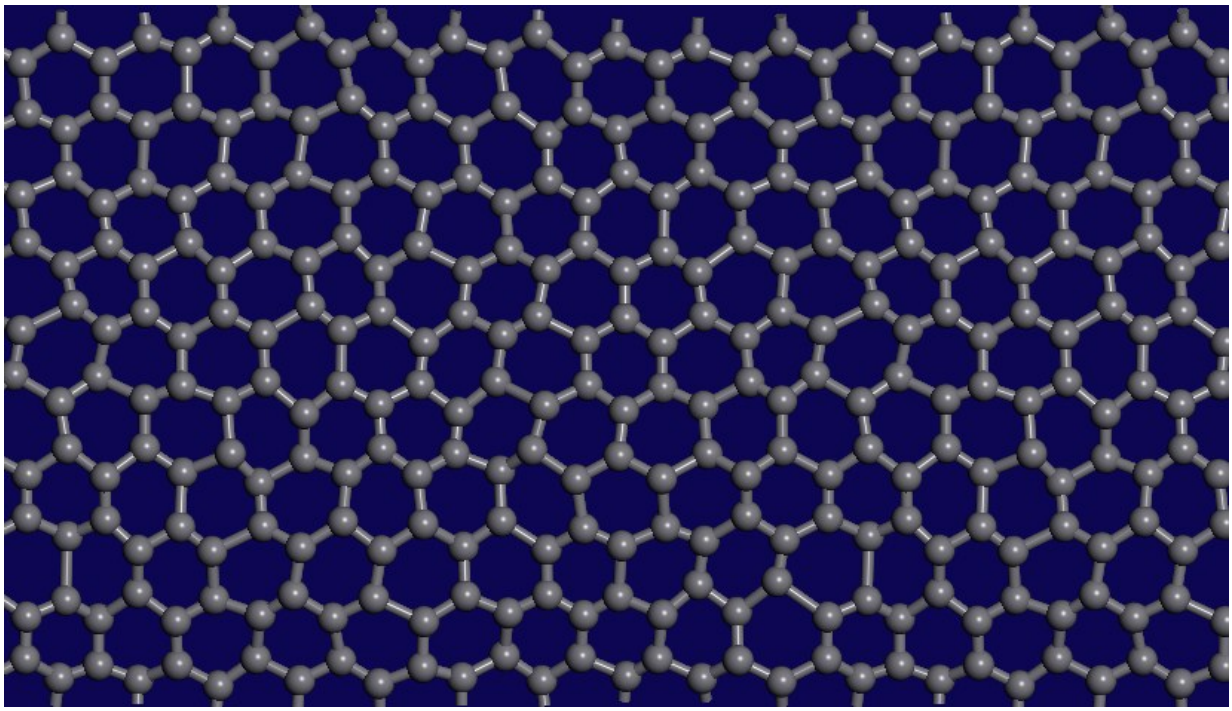

Figure S3. Last frame of the 4500 K simulation, top view.

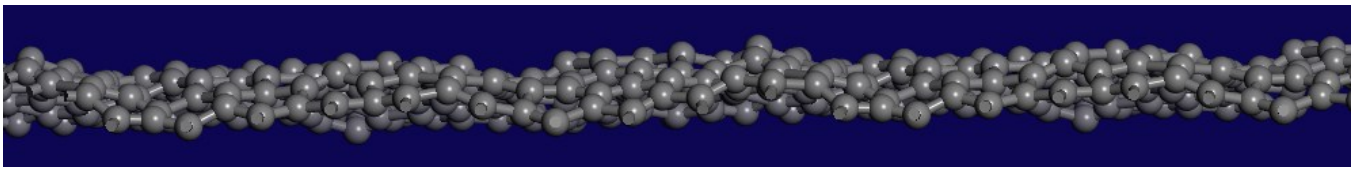

Figure S4. Last frame of the 4500 K simulation, side view.

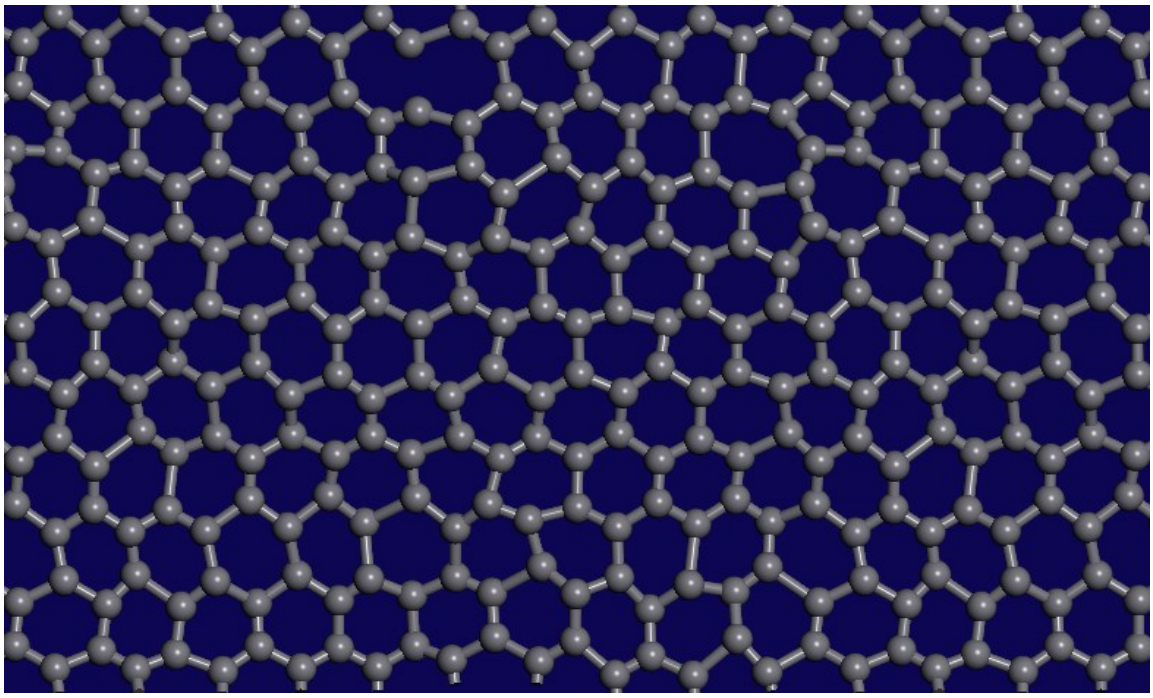

Figure S5. Last frame of the 5000 K simulation, top view.

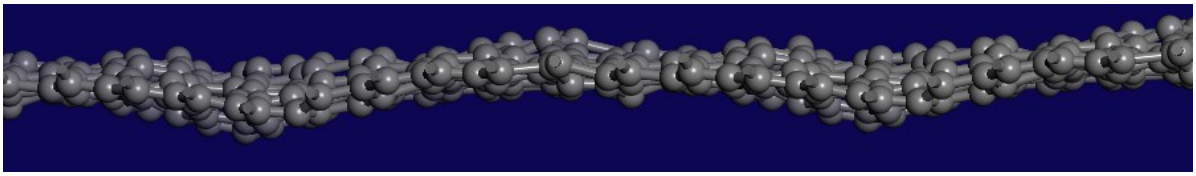

Figure S6. Last frame of the 5000 K simulation, side view.

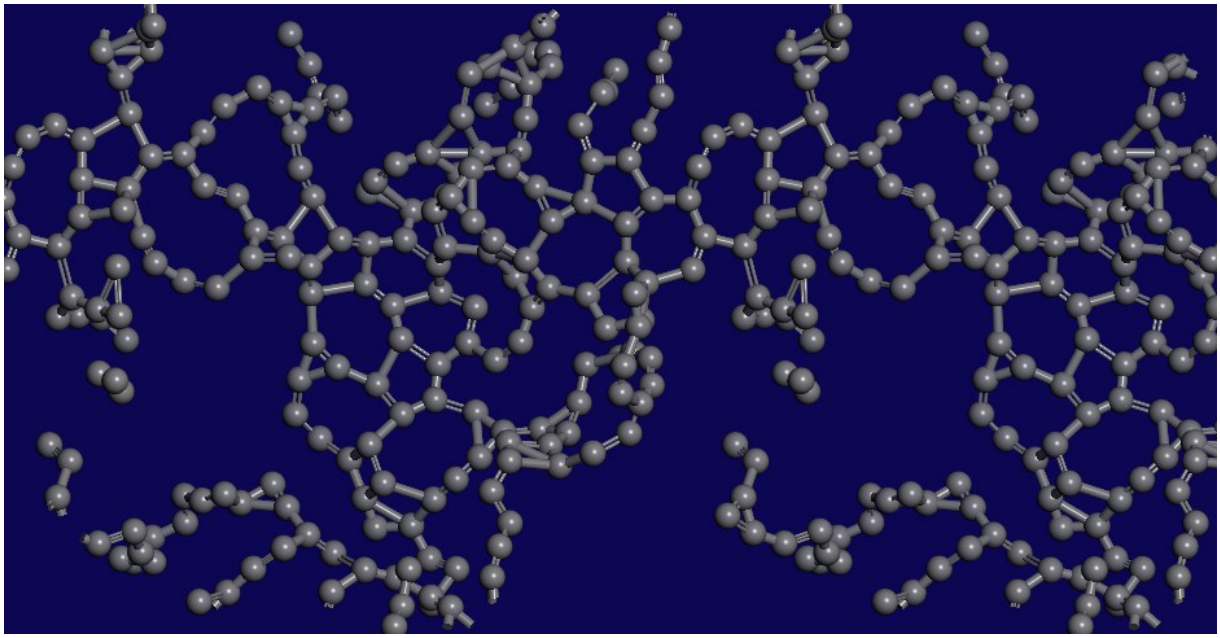

Figure S7. Last frame of the 6000 K simulation, top view.

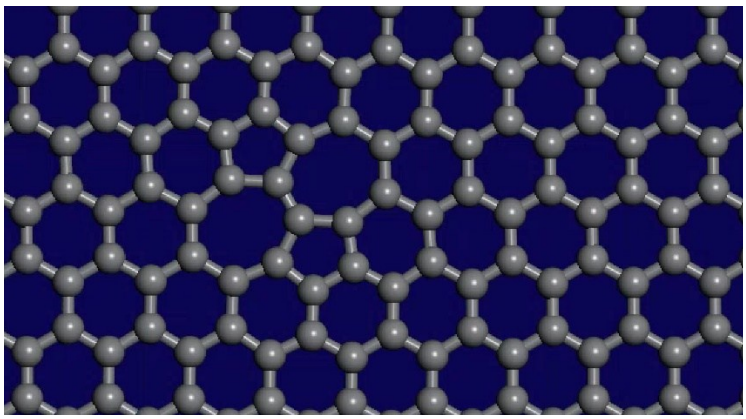

Figure S8. Flat 5775 defect in 10x10 cell at 0 K (top view).

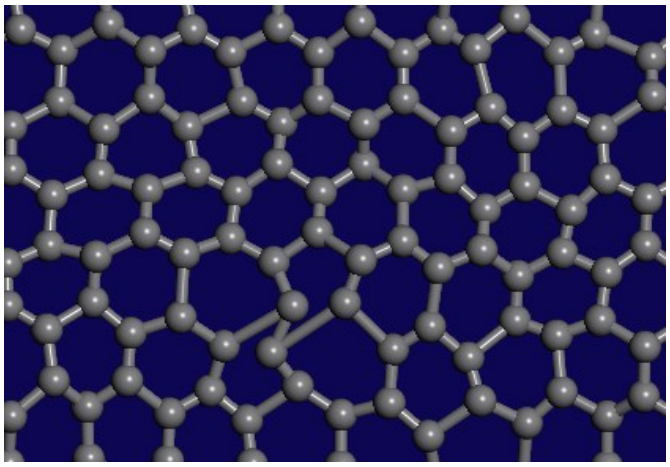

Figure S9. Last frame of 5000 K simulation. We have not rebonded so that one can see the net motion of the atoms that has occurred, which results in the formation of a single 5775 defect at the bottom left. Two atoms have rotated in place.

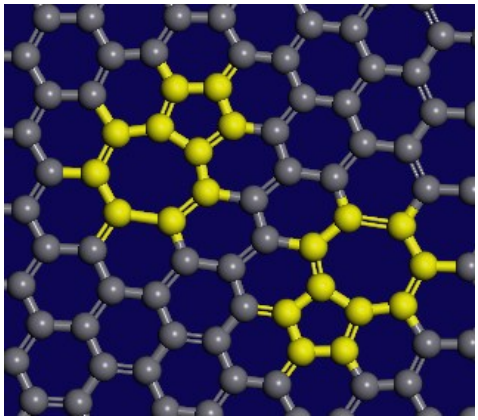

Figure S10. Separated 57 and 75 defects (Flat).

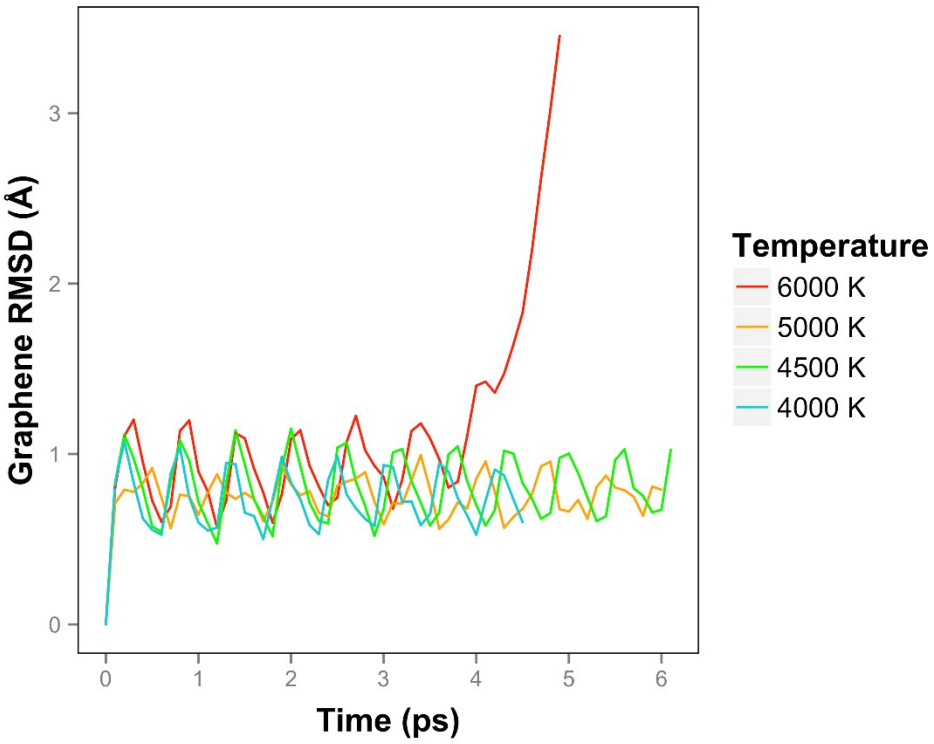

Figure S11. Root mean squared displacement (RMSD) vs. time for 4 temperatures.

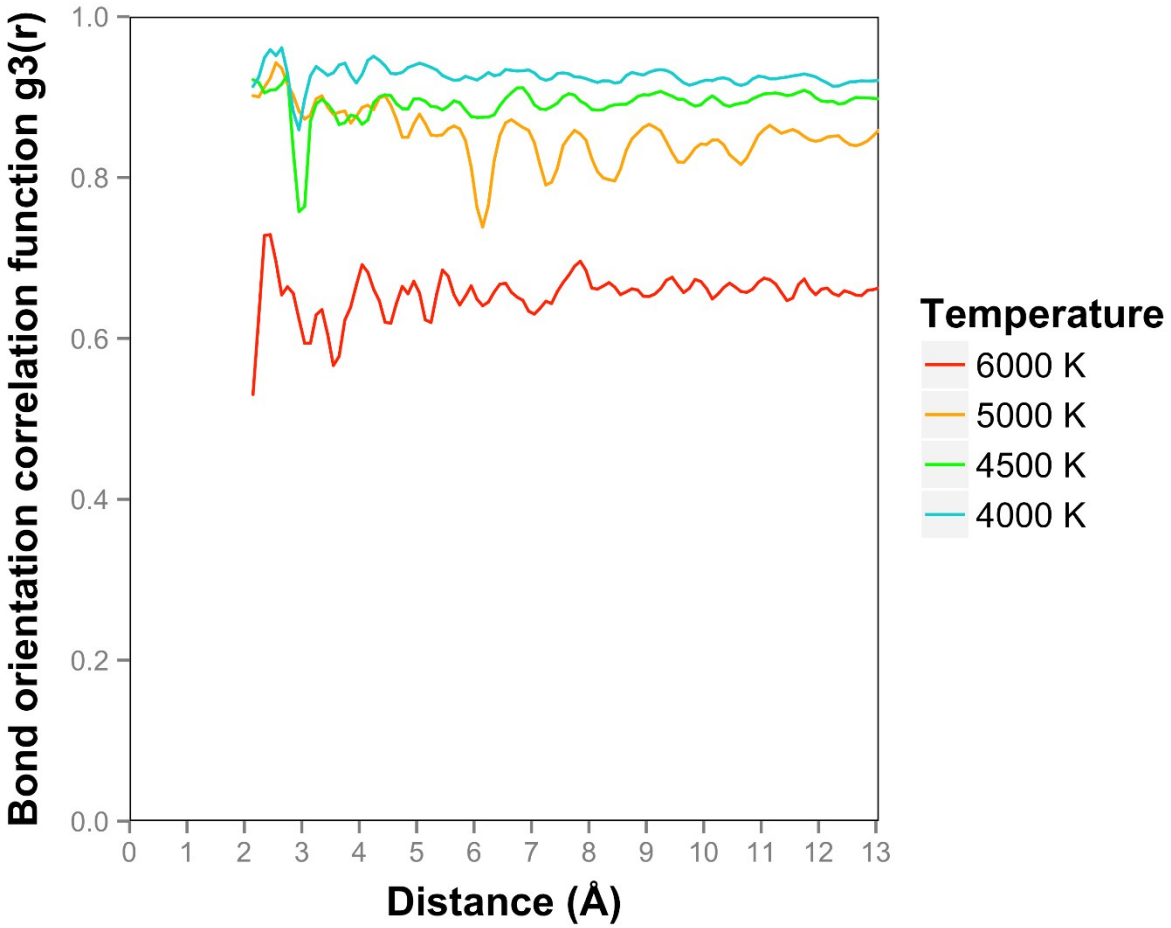

Figure S12: Bond orientation correlation function as a function of distance at 4 temperatures.

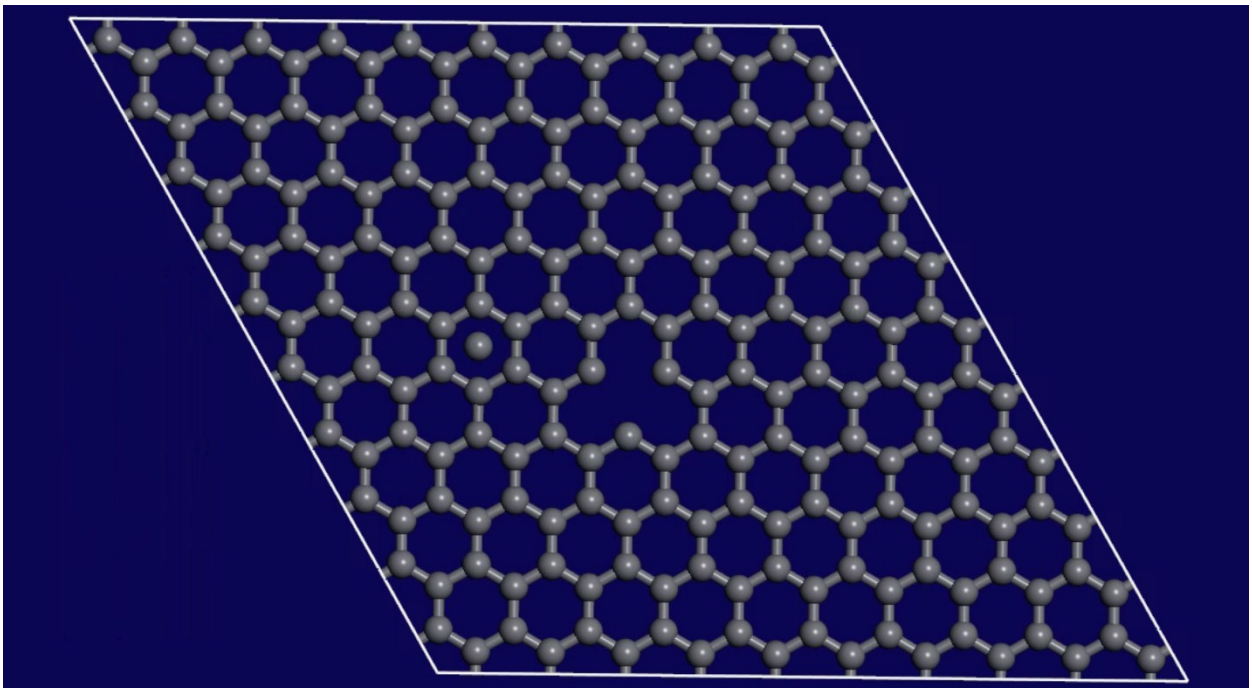

Figure S13. 10 x 10 graphene unit cell with 1 C atom removed from lattice to form an adatom and a single vacancy defect. This system was then run for 6 ps MD to test for reduced melting point.

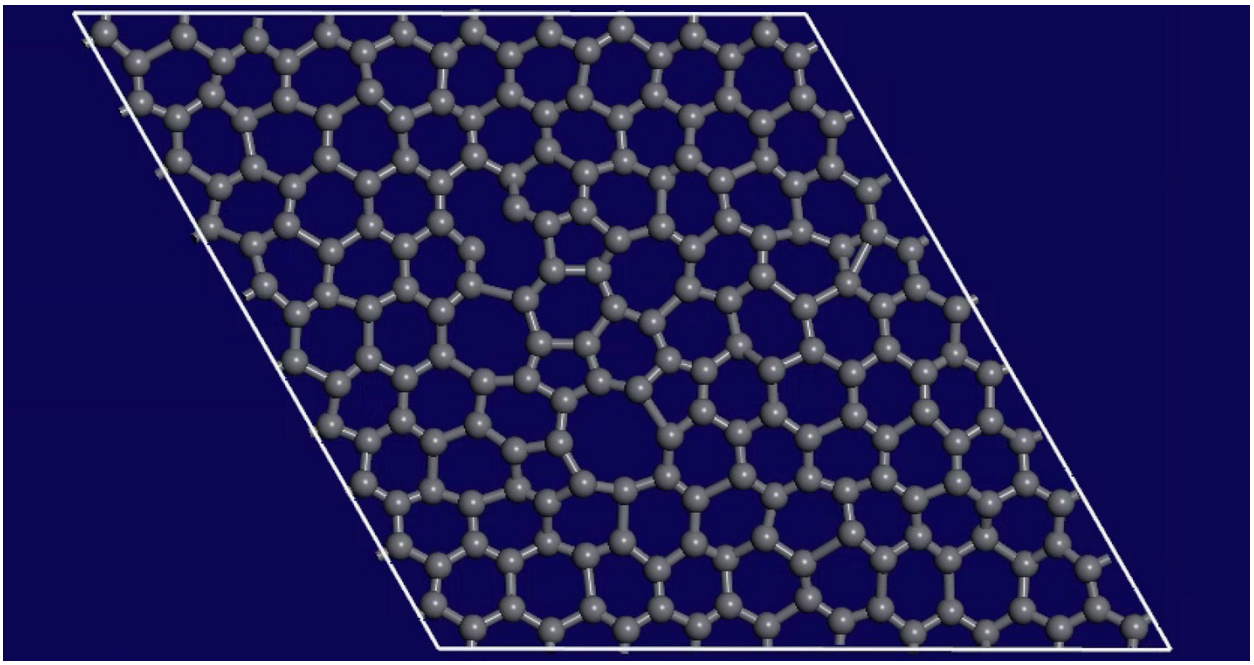

Figure S14. Result of 6.2 ps annealing at 4500 K. Starting from defect configuration shown in Figure S13. We observe that the system is in a quasi-2D liquid state. The adatom has annealed out leaving relatively stable 57, 75, and 585 defects within 1 ps, which persisted for 5 ps (The remaining duration of the

simulation). This final snapshot also shows a 3-ring and a broken bond (10-ring), which are temporary excitations.

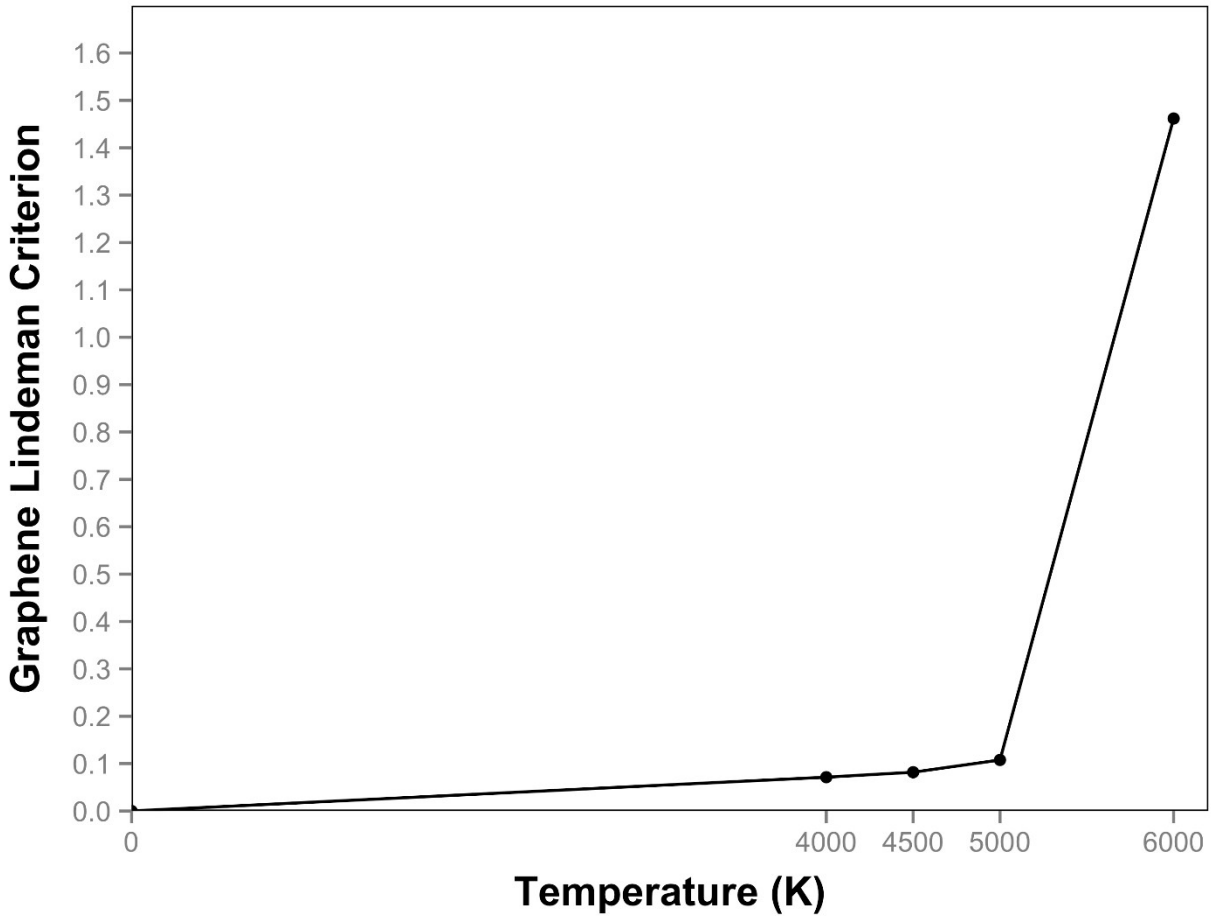

Figure S15. Lindemann criterion results between 0 K and 6000 K.