Imaging the C Black Formation by Acetylene Pyrolysis with Molecular Reactive Force Field Simulations

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Electronic Supplementary Information (ESI)

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s1. Comparison of pyrolysis evolutions under various conditions.

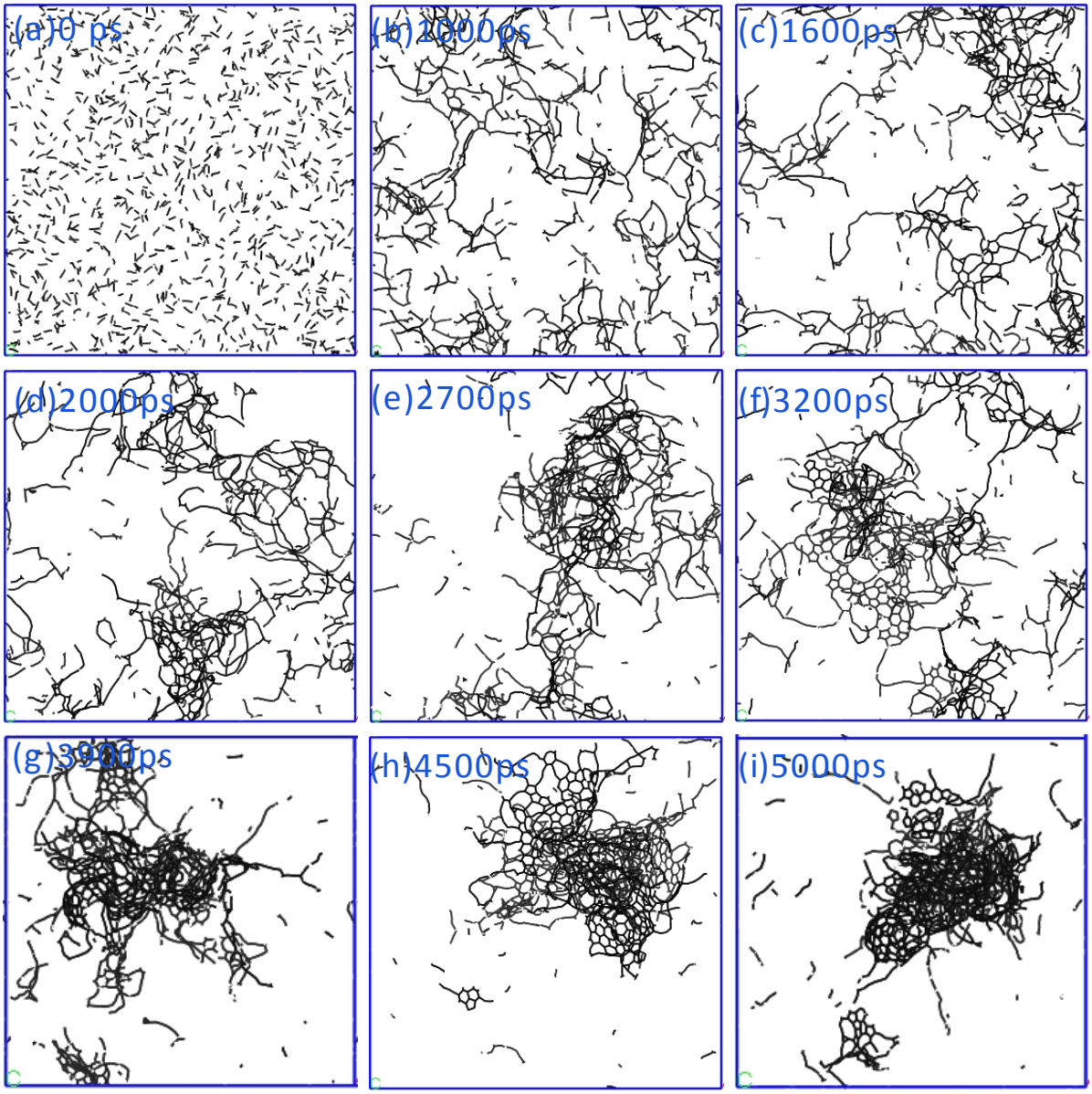

Fig. s1 Snapshots of acetylene pyrolysis as time proceeds under the condition of 0.1g/cm^3 and 3000 K. Only carbon atoms are exhibited. (a)-(i) correspond to 0, 1000, 1600, 2000, 2700, 3200, 3900, 4500 and 5000 ps, respectively.

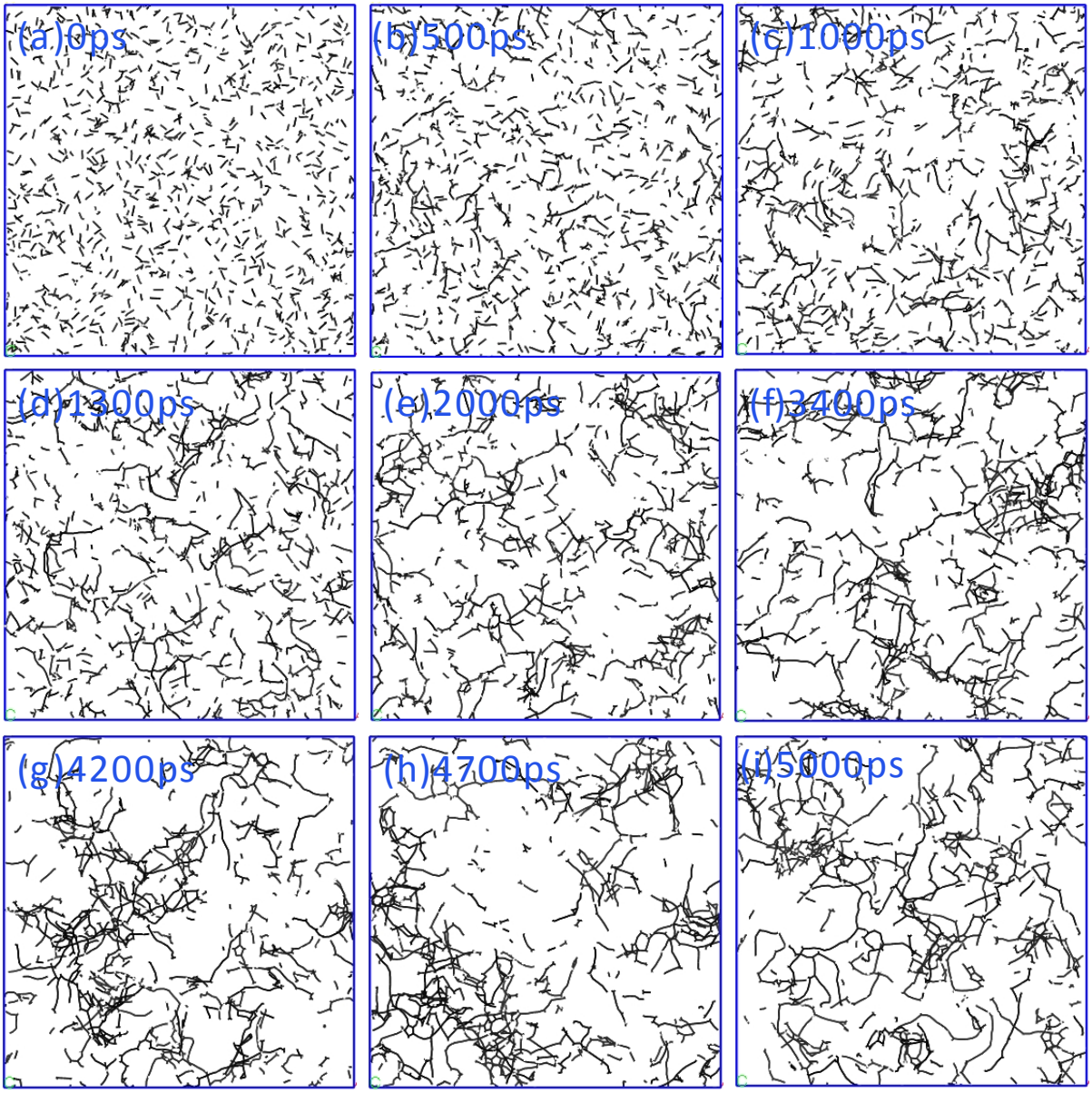

Fig. s2 Snapshots of acetylene pyrolysis as time proceeds under the condition of 0.1g/cm^3 and 2500 K. Only carbon atoms are exhibited. (a)-(i) correspond to 0, 500, 1000, 1300, 2000, 3400, 4200, 4700 and 5000 ps, respectively.

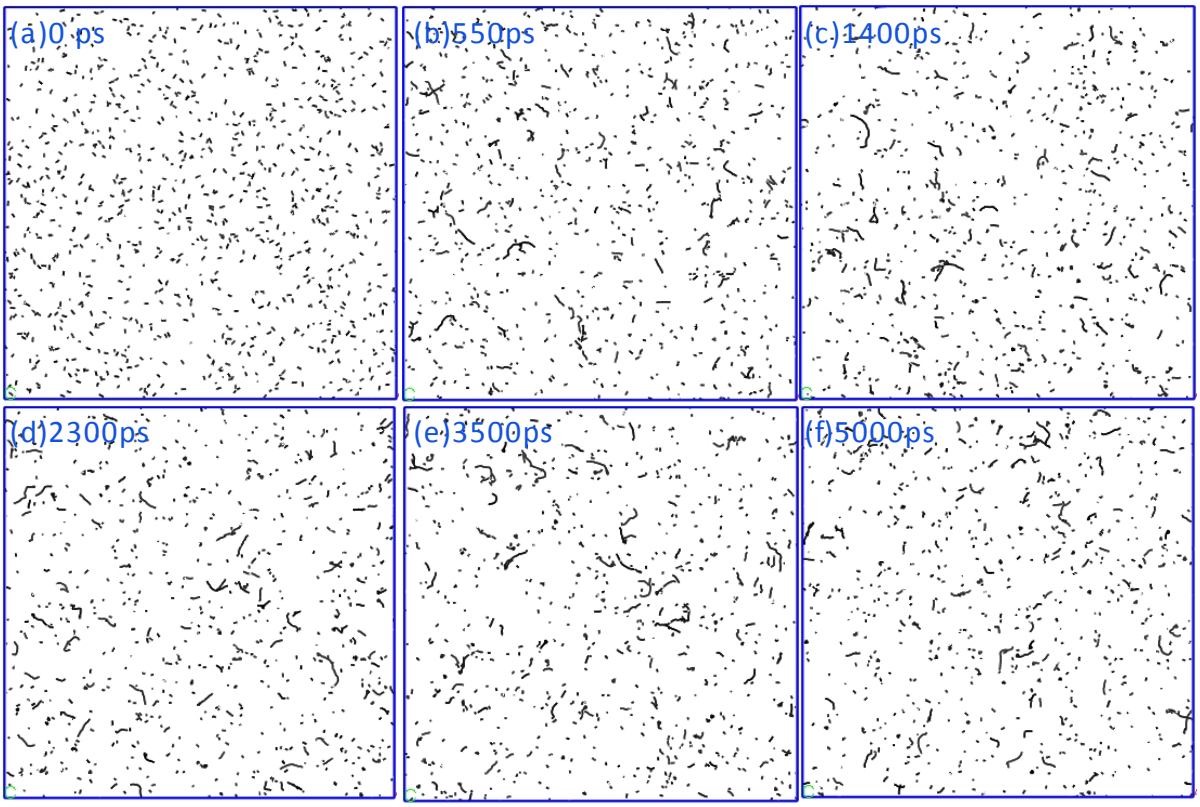

Fig. s3 Snapshots of acetylene pyrolysis as time proceeds under the condition of 0.01g/cm^3 and 3500 K. Only carbon atoms are exhibited. (a)-(f) correspond to 0, 550, 1400, 2300, 3500 and 5000 ps, respectively.

Comparing the snapshots in Figs. s1-s3 with those in Fig. 2 of text, we find that the evolution processes under various conditions of densities and temperatures are similar, only with a difference of the evolution velocity. Therefore, we can employ the result of 0.1 g/cm3 and 3500 K for discussion, because the evolution tends to balance within the time limitation of simulations.

s2. Evolution of C11-C20 under the condition of 0.1 g/cm^3 and 3500 K

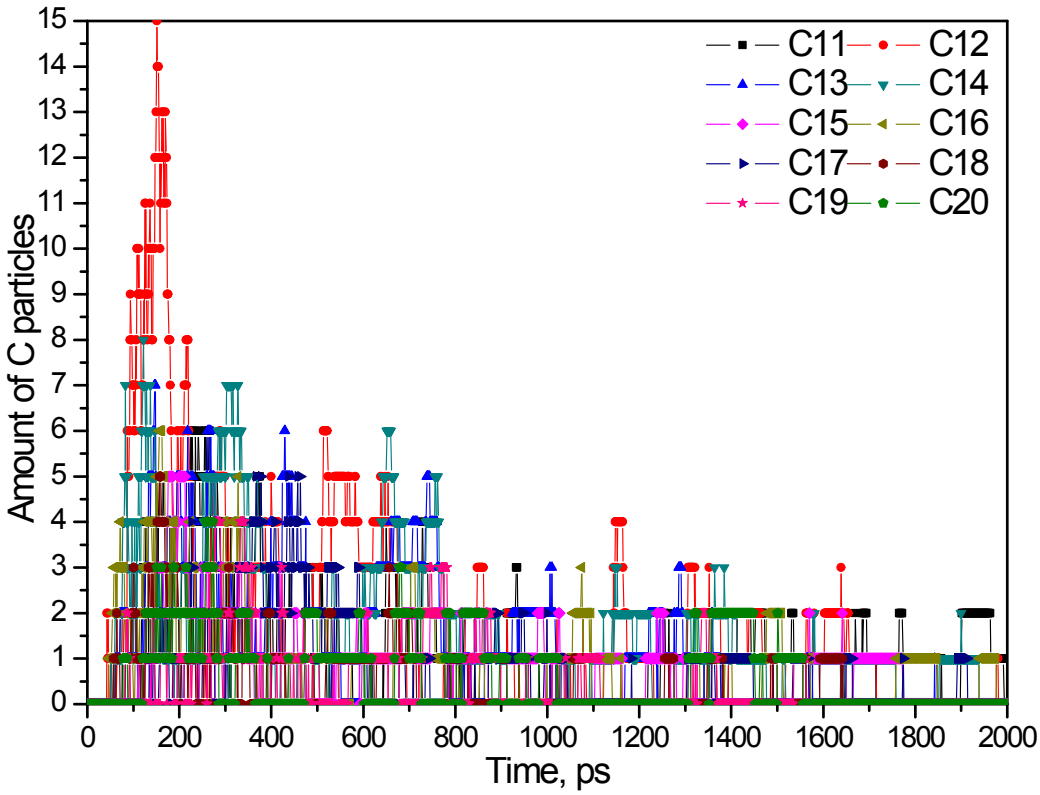

Fig. s4 Evolution of C11-C20 particles under the condition of 0.1 g/cm^3 and 3500 K.

s3. Evolution of C4, C6 particles under the condition of 0.01 g/cm^3.

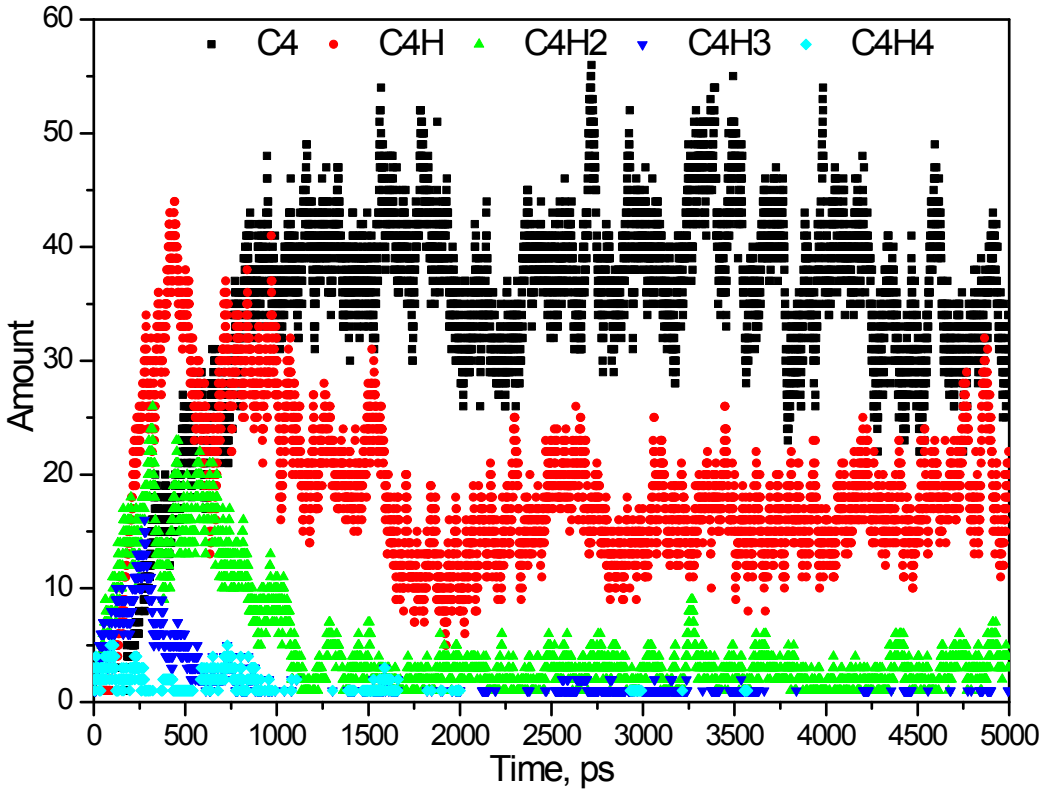

Fig. s5 Evolution of C4 under the condition of 0.01 g/cm^3 and 3500 K.

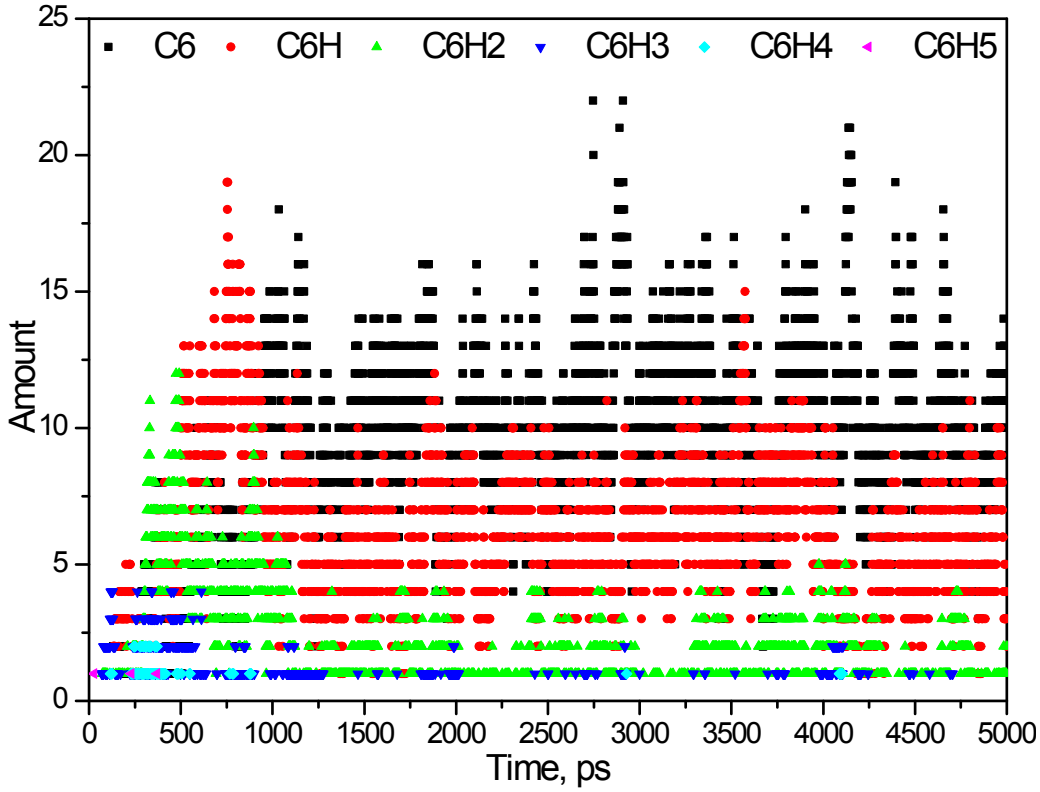

Fig. s6 Evolution of C6 under the condition of 0.01 g/cm^3 and 3500 K.

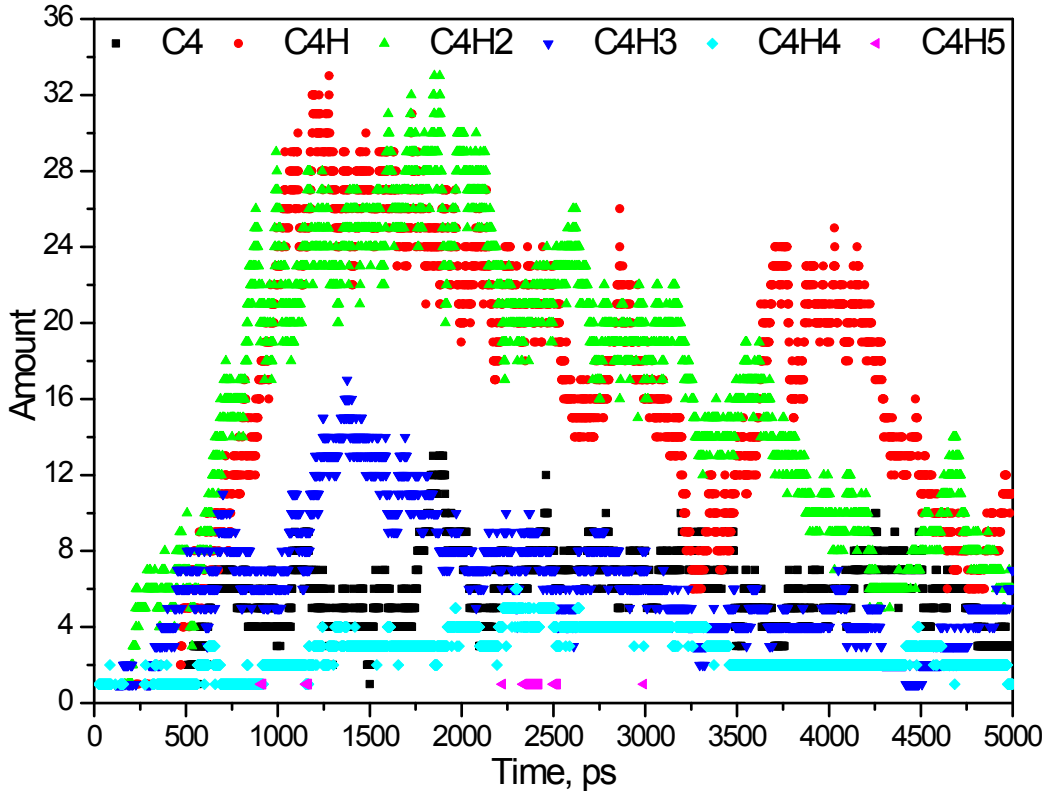

Fig. s7 Evolution of C4 under the condition of 0.01 g/cm^3 and 2500 K.

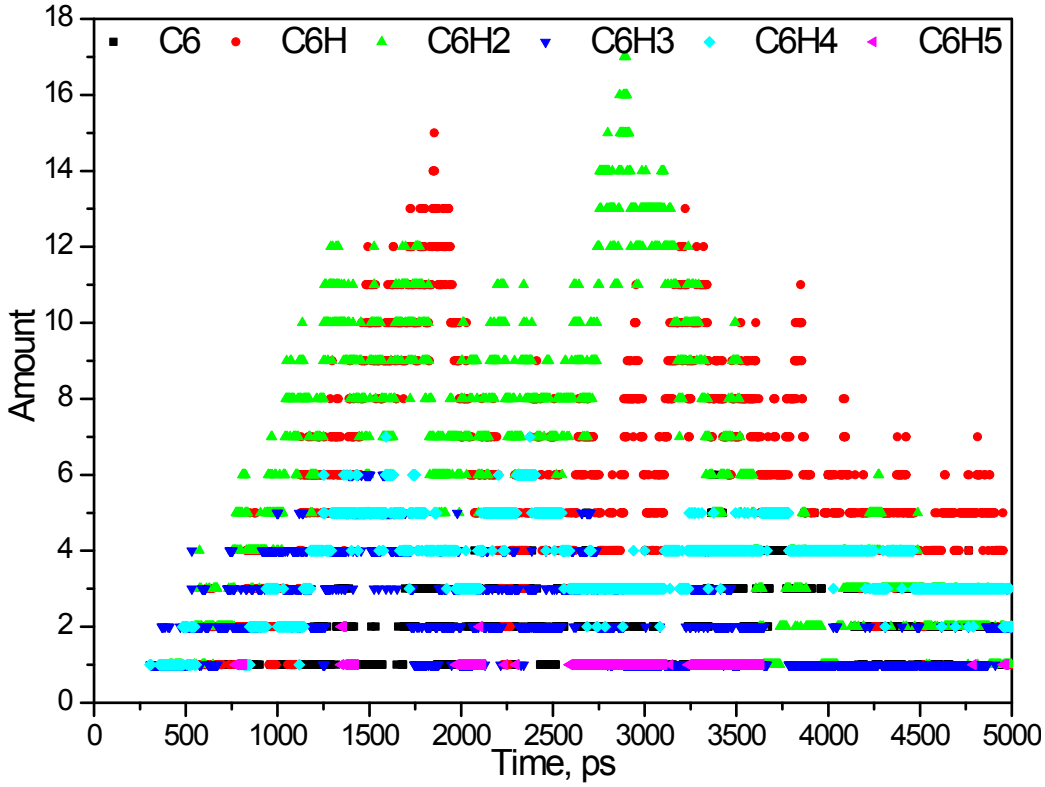

Fig. s8 Evolution of C6 under the condition of 0.01 g/cm^3 and 2500 K.

s4. Evolution of total amount of all C particles under different conditions.

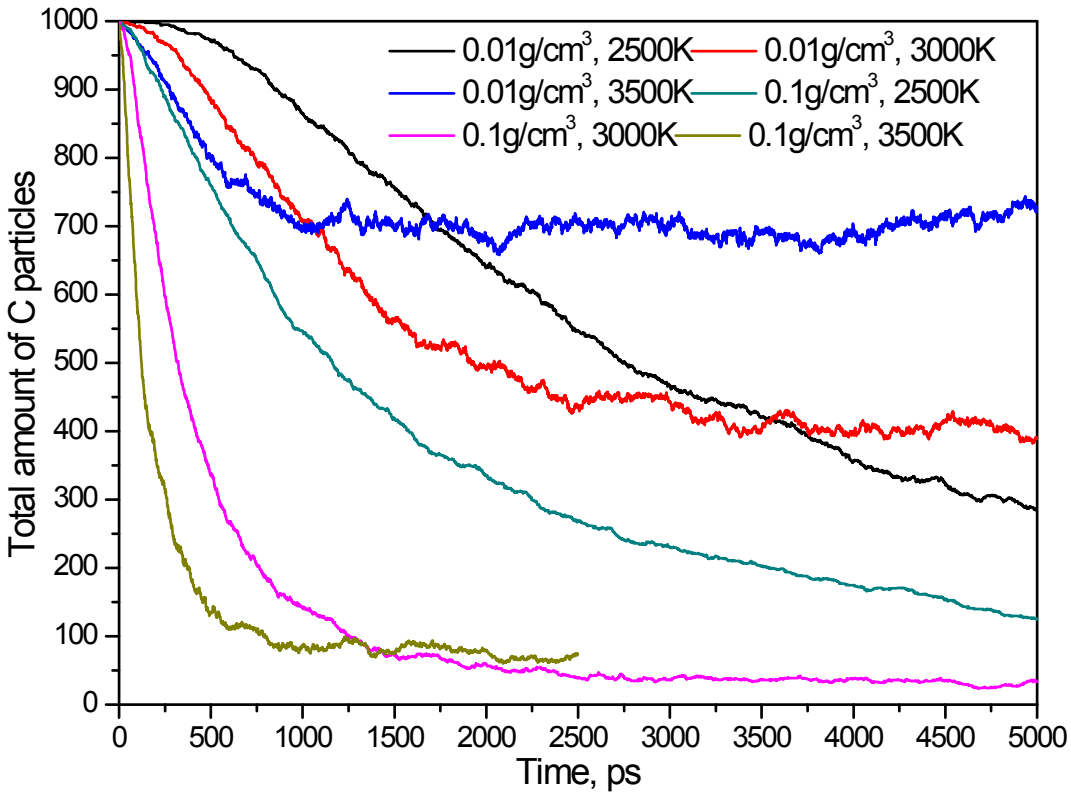

Fig. s9 Evolution of total amount of all C particles under different conditions.