

Supplementary Information for

Oxidation of Graphene with Variable Defects: Alternately Symmetrical Escape and Self-restructuring of Carbon Rings

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Figure S1 to S6

Caption for Video S1

Figure S1 to S6

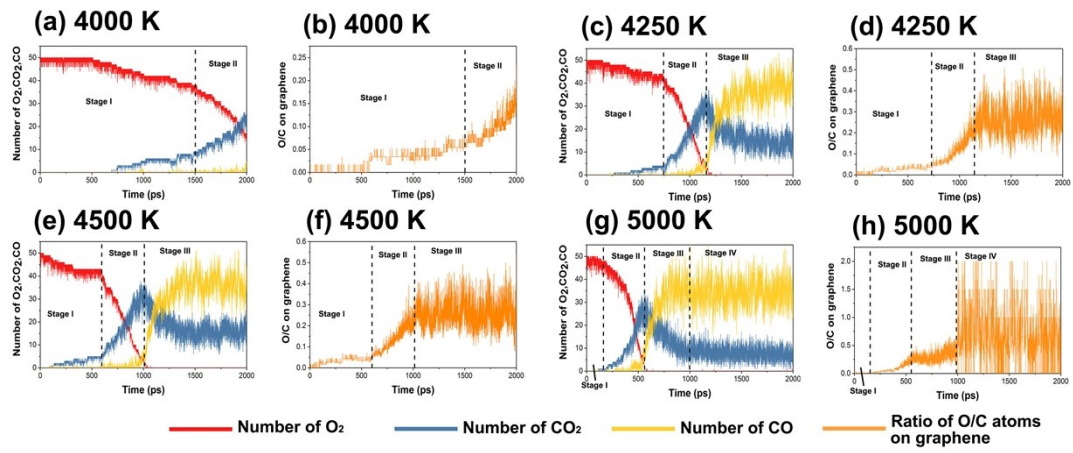


Figure S1. Quantity changes of gases and ratio of O/C on the SVD graphene within 2 ps at (a) (b) 4000 K (c) (d) 4250 K (e) (f) 4500 K (g) (h) 5000 K.

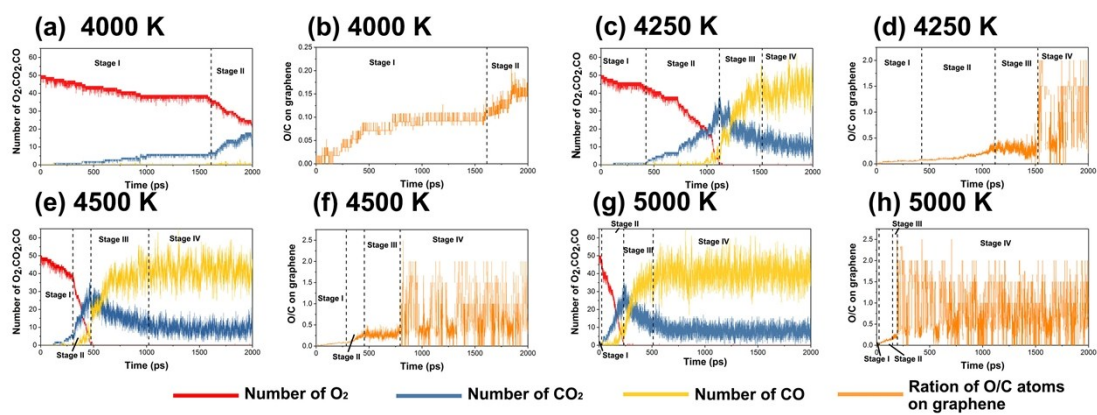


Figure S2. Quantity changes of gases and ratio of O/C on the MVD graphene within 2 ps at (a) (b) 4000 K (c) (d) 4250 K (e) (f) 4500 K (g) (h) 5000 K.

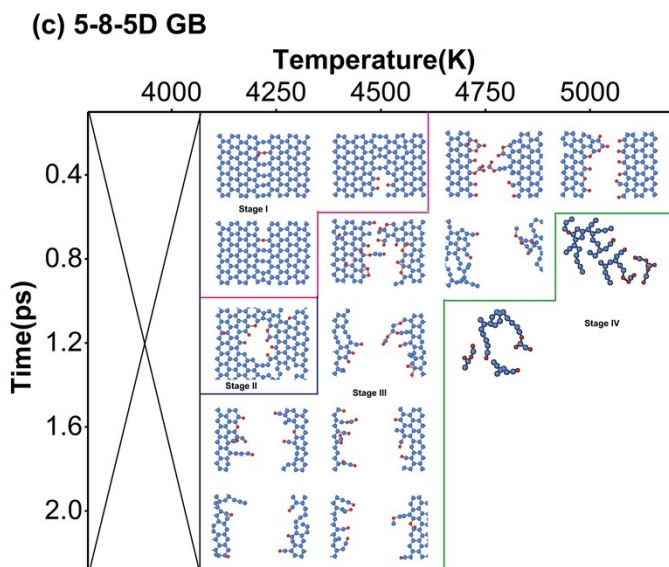
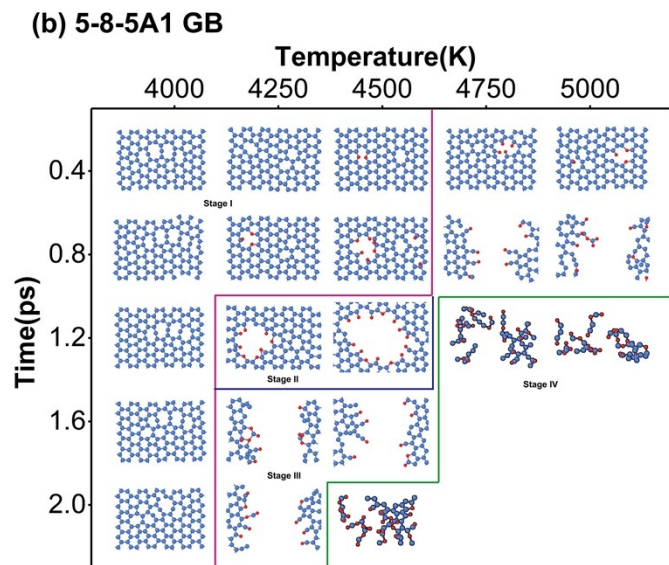
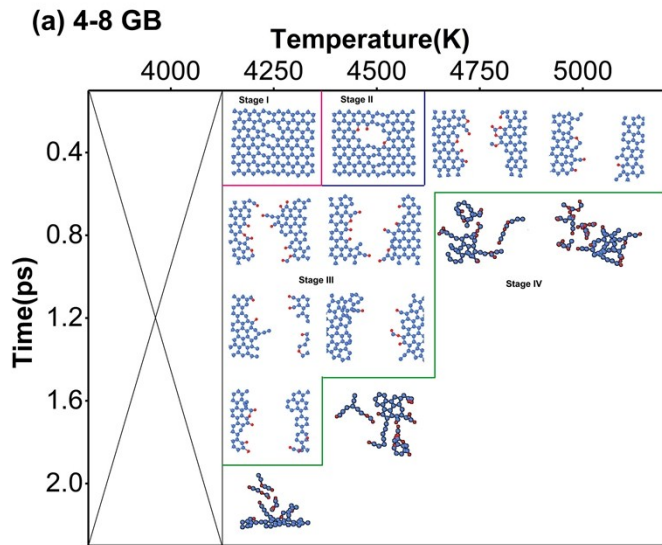


Figure S3. Structural phase diagram of the (a) 4-8 GB graphene (b) 5-8-5A1 GB graphene and (c) 5-8-5D GB graphene oxidation stage. Stages are separated from each other by full lines with different colors. 4-8 GB and 5-8-5D graphene sheets were not oxidized at 4000 K within 2 ps so that we filled the corresponding part of the diagram with an “X”.

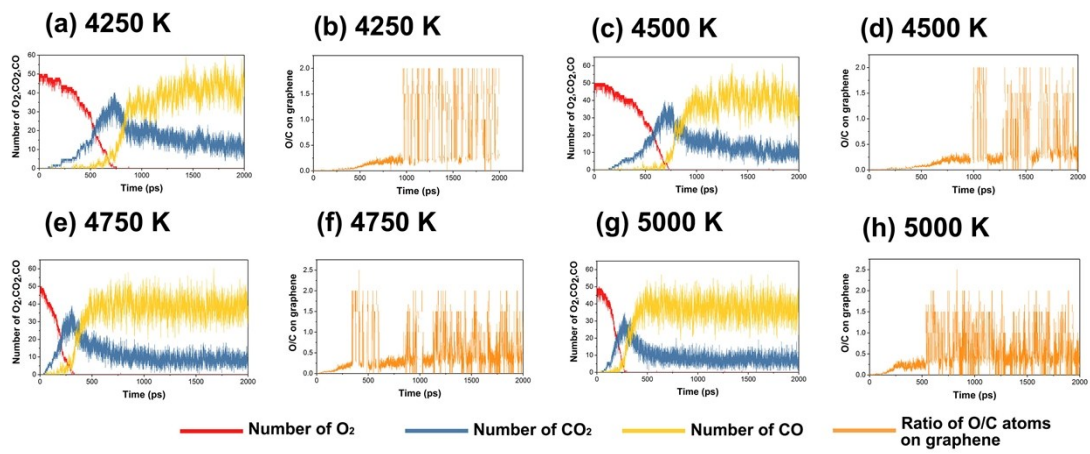


Figure S4. Quantity changes of gases and ratio of O/C on the 4-8 GB graphene within 2 ps at (a) (b) 4250 K (c) (d) 4500 K (e) (f) 4750 K (g) (h) 5000 K.

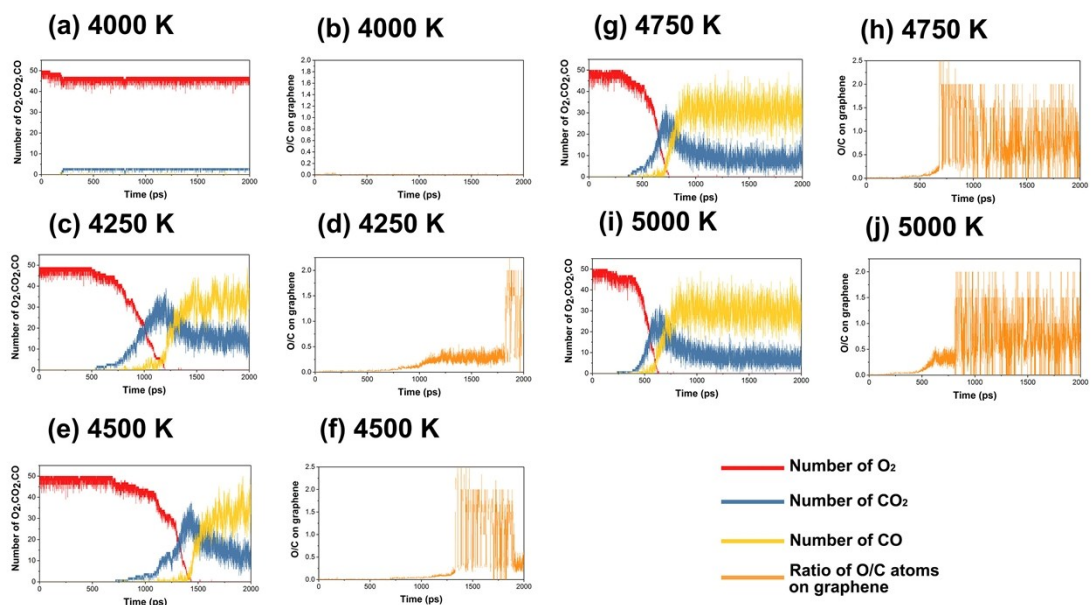


Figure S5. Quantity changes of gases and ratio of O/C on the 5-8-5A1 GB graphene within 2 ps at (a) (b) 4250 K (c) (d) 4250 K (e) (f) 4500 K (g) (h) 4750 K (i) (j) 5000 K.

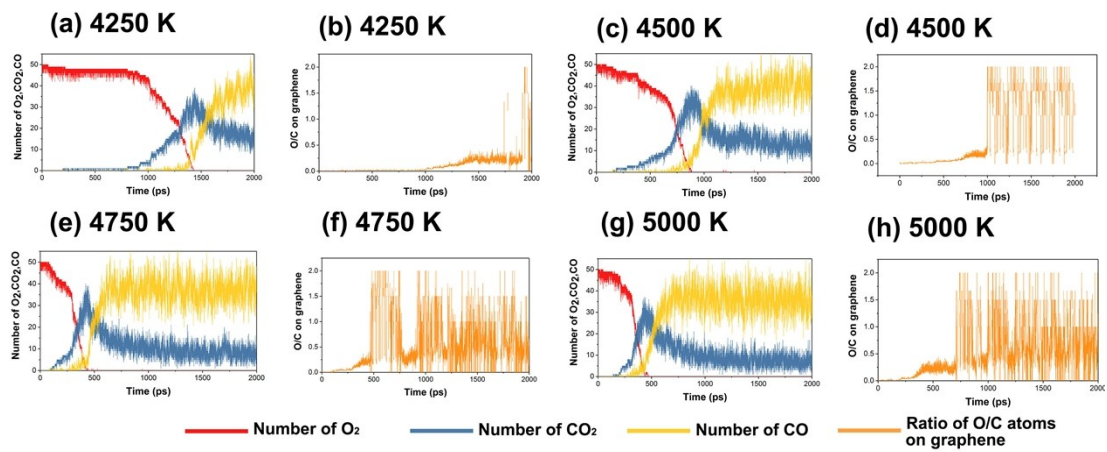


Figure S6. Quantity changes of gases and ratio of O/C on the 5-8-5D GB graphene within 2 ps at (a) (b) 4250 K (c) (d) 4500 K (e) (f) 4750 K (g) (h) 5000 K.

Caption for Video S1

Video S1. Symmetrical escape of C atoms in stage I on SVD graphene. During stage I on the SVD graphene, we found the symmetry of the vacancy was preserved