

Study on the Thermal Decomposition Mechanism of Graphene Oxide Functionalized with Triaminoguanidine (GO-TAG) by Molecular Reactive Dynamics and Experiments

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The parallel calculation of TAG and GO-TAG decomposition kinetics were shown in Figure S1, Figure S2 and Figure S3. The results are in good agreement, with little errors.

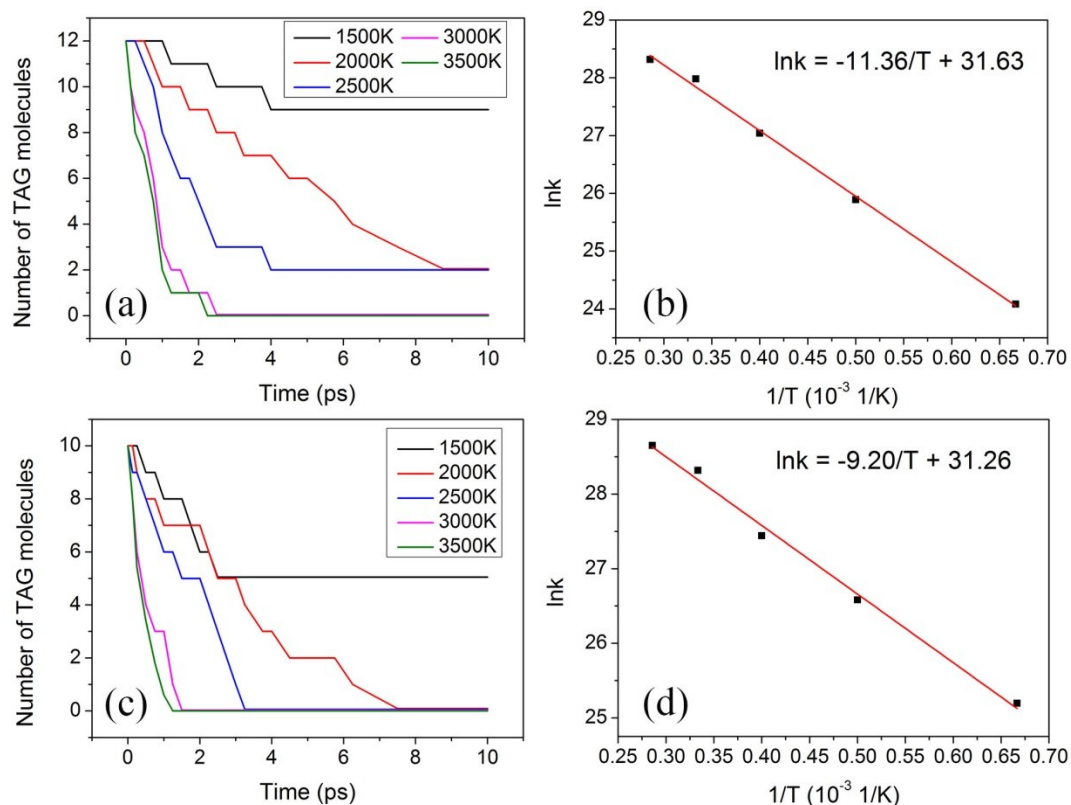


Figure S1. (a) Evolution of the pure TAG molecules over time at various temperatures; (b) Arrhenius plot of the rate constants of pure TAG molecules at various temperatures; (c) evolution of TAG molecules over time at various temperatures in GO-TAG; (d) Arrhenius plot of the rate constants of TAG molecules at various temperatures in GO-TAG.

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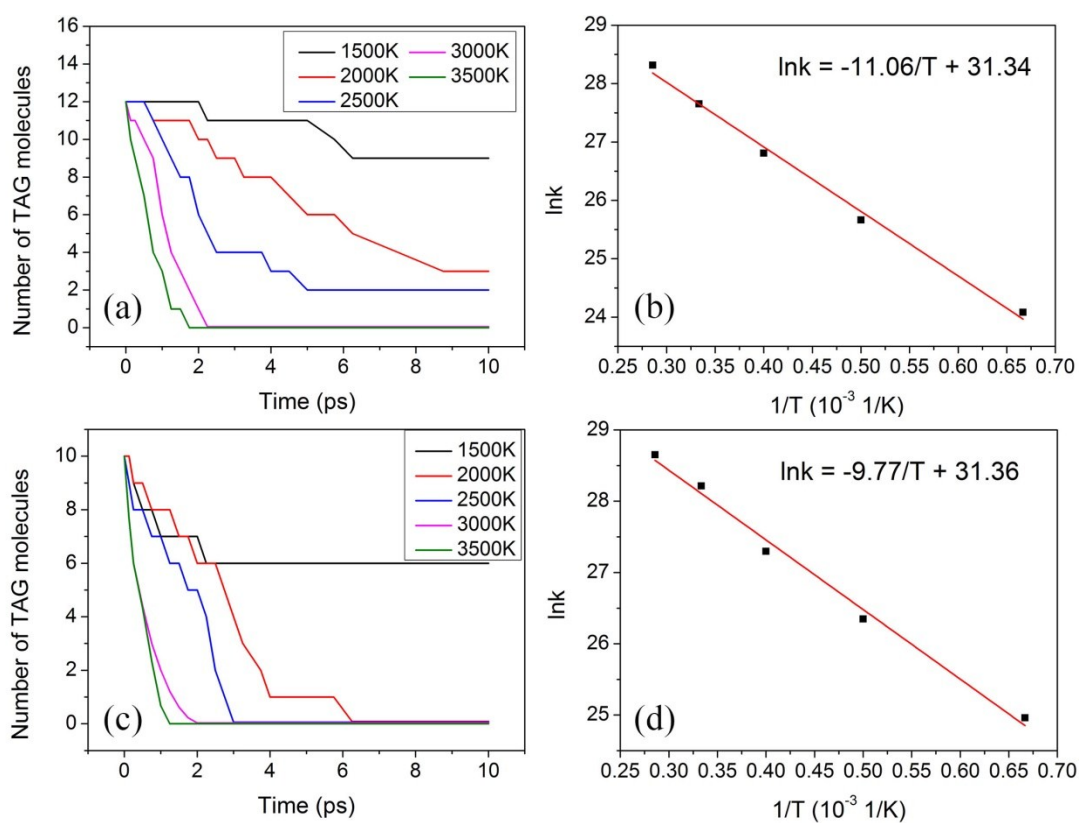


Figure S2. (a) Evolution of the pure TAG molecules over time at various temperatures; (b) Arrhenius plot of the rate constants of pure TAG molecules at various temperatures; (c) evolution of TAG molecules over time at various temperatures in GO-TAG; (d) Arrhenius plot of the rate constants of TAG molecules at various temperatures in GO-TAG.

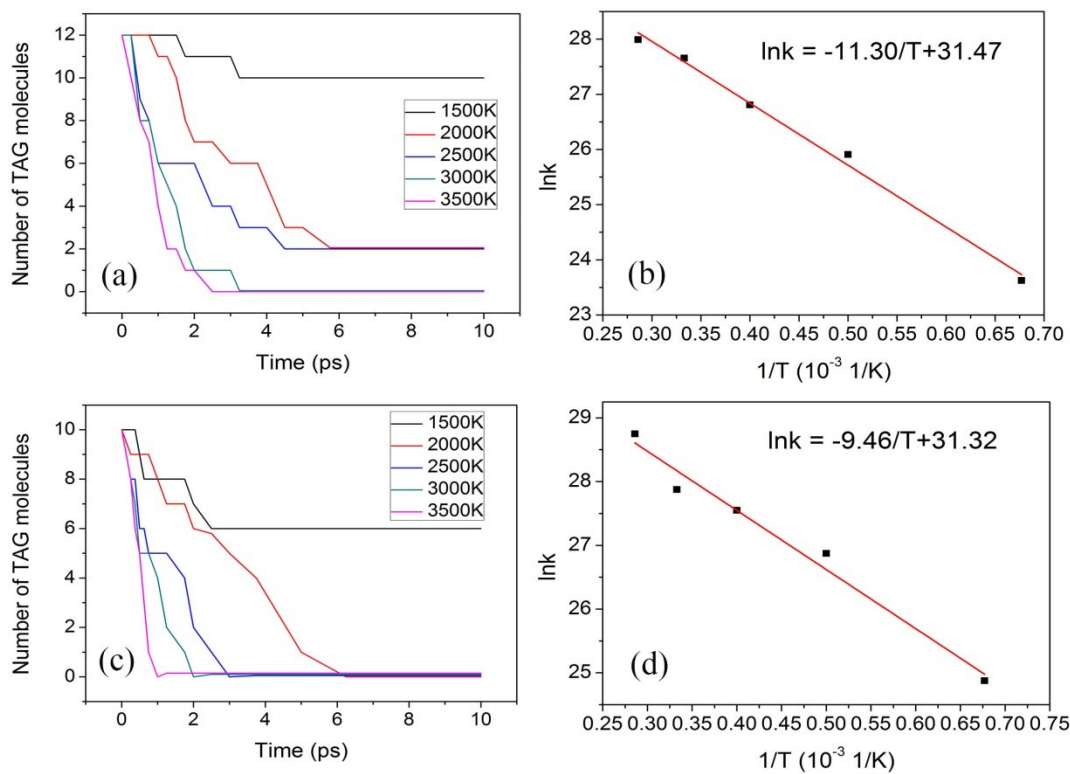


Figure S3. (a) Evolution of the pure TAG molecules over time at various temperatures; (b) Arrhenius plot of the rate constants of pure TAG molecules at various temperatures; (c) evolution of TAG molecules over time at various temperatures in GO-TAG; (d) Arrhenius plot of the rate constants of TAG molecules at various temperatures in GO-TAG.

The decomposition movies of TAG and GO-TAG are attached here as a supplement to Figure 8 and Figure 9.



TAG.mp4



GO-TAG-1.avi