Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Molecular Dynamics Simulation Reveals How Graphene Oxide Stabilizes and Activates Lipase in an Anhydrous Gas

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SI 1. Force-field parameters

Table S1. Nonbonding parameters for GO

Type	*Mass*	*Charge*	*Sigma*(nm)	*Epsilon*(kJ mol^{-1} nm^{-2})
CA(opls_166)	12.0110	0.150	3.55000e-01	2.92880e-01
CT(opls_182)	12.0110	0.140	3.50000e-01	2.76144e-01
C(opls_267)	12.0110	0.520	3.75000e-01	4.39320e-01
CA(opls_147)	12.0110	0.000	3.55000e-01	2.92880e-01
HO(opls_168)	1.0080	0.435	0.00000e+00	0.00000e+00
HO(opls_270)	1.0080	0.450	0.00000e+00	0.00000e+00
OH(opls_167)	15.9994	-0.585	3.07000e-01	7.11280e-01
OH(opls_268)	15.9994	-0.530	3.00000e-01	7.11280e-01
O_3(opls_269)	15.9994	-0.440	2.96000e-01	8.78640e-01
OS(opls_179)	15.9994	-0.280	2.90000e-01	5.85760e-01

Table S2. Bond stretching parameters for GO

Type *i*	Type *j*	*func*	b_0(nm)	k_b(kJ mol^{-1} nm^{-2})
CA	CA	1	0.14000	392459.2
CT	CT	1	0.15290	224262.4
CA	CT	1	0.15100	265265.6
C	CA	1	0.14900	334720.0
C	CT	1	0.15220	265265.6
CA	OH	1	0.13640	376560.0
OH	HO	1	0.09450	462750.4
CT	OS	1	0.14100	267776.0
C	OH	1	0.13640	376560.0
C	O_3	1	0.12290	476976.0

Table S3. Angle bending parameters for GO

Type *i*	Type *j*	Type *k*	*func*	θ_0 (deg)	k_θ (kJ mol^{-1} rad^{-2})
CT	OS	CT	1	109.500	502.080
C	OH	HO	1	113.00	292.880
CA	OH	HO	1	113.00	292.880
CA	CA	CA	1	120.000	527.184
CT	CT	CA	1	114.000	527.184
CA	CT	CA	1	109.500	334.720
CT	CA	CT	1	116.000	585.760
C	CT	CA	1	112.000	527.184
CT	CT	C	1	111.100	527.184
CA	CA	OH	1	120.000	585.760
CA	CT	OS	1	109.500	418.400
C	CT	OS	1	109.500	418.400
CT	C	O_3	1	120.400	669.440
CT	C	OH	1	108.000	585.760
CA	C	O_3	1	120.400	669.440
CA	C	OH	1	120.000	585.760
O_3	C	OH	1	121.000	669.440
CT	CA	CA	1	120.000	585.760
C	CA	CA	1	120.000	711.280
CA	CA	CT	1	119.700	585.760

Table S4. Dihedral potential parameters for GO

Type *i*	Type *j*	Type *k*	Type *l*	*func*	C_0	C_1	C_2	C_3	C_4	C_5
CA	CT	OS	CT	3	1.71544	2.84512	1.04600	-5.60656	0.0000	0.0000
C	CT	OS	CT	3	1.71544	2.84512	1.04600	-5.60656	0.0000	0.0000
CA	CA	CT	OS	3	0.00000	0.00000	0.00000	0.00000	0.0000	0.0000
CA	CA	OH	HO	3	7.03749	0.00000	-7.03749	0.00000	0.0000	0.0000
HO	OH	C	O_3	3	23.0120	0.00000	-23.0120	0.00000	0.0000	0.0000
CA	CA	C	O_3	3	8.78640	0.00000	-8.78640	0.00000	0.0000	0.0000
CA	CA	C	OH	3	8.78640	0.00000	-8.78640	0.00000	0.0000	0.0000
CA	C	OH	HO	3	29.2880	-8.3680	-20.9200	0.00000	0.0000	0.0000
CT	C	OH	HO	3	26.1500	-3.1380	-23.0120	0.00000	0.0000	0.0000
CA	CA	CA	CT	3	30.3340	0.00000	-30.3340	0.00000	0.0000	0.0000
CA	CT	CT	CA	3	30.3340	0.00000	-30.3340	0.00000	0.0000	0.0000
CT	CA	CA	CA	3	30.3340	0.00000	-30.3340	0.00000	0.0000	0.0000
CA	CA	CT	CT	3	30.3340	0.00000	-30.3340	0.00000	0.0000	0.0000
CA	CA	CA	CA	3	30.3340	0.00000	-30.3340	0.00000	0.0000	0.0000

SI 2. Validation of the simulated annealing procedure

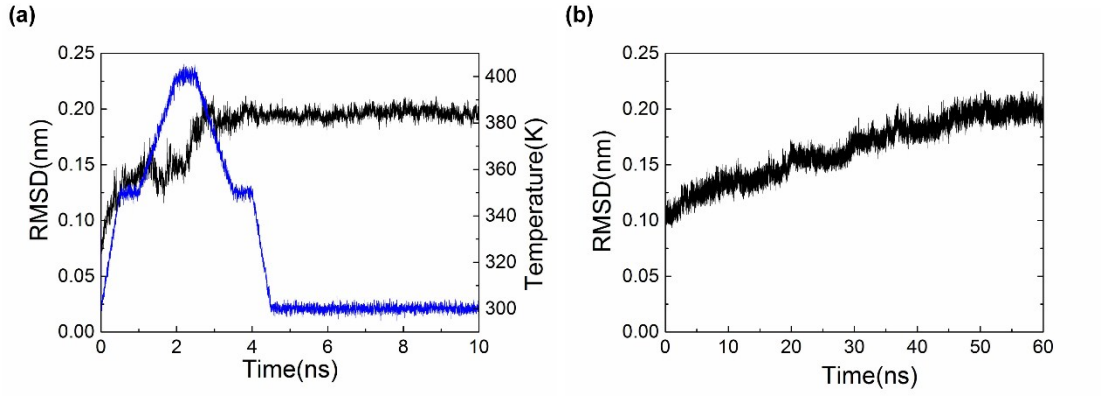

Fig. S1 (a) RMSD of CALB backbone under the simulated annealing procedure. (b) RMSD of CALB backbone with molecular dynamic simulation in an NVT ensemble.

SI 3. Analysis of the conformation fluctuations of the GO

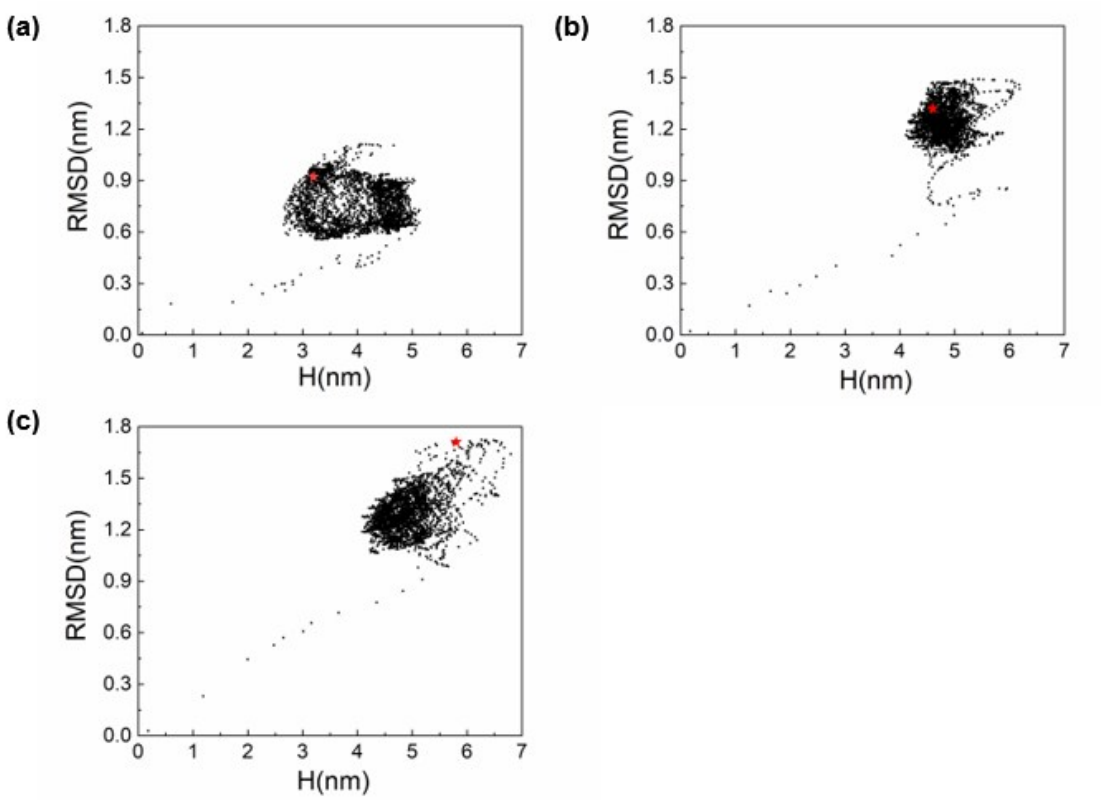

Fig. S2 The conformational fluctuations of (a) LGO, (b) MGO and (c) HGO. Black dots represent the RMSD of the GO sheet and height (the distance between the highest point and the lowest point of the GO sheet) at each moment without CALB. Red dot represents the RMSD and height of the GO sheet after CALB and GO assembly.

SI 4. Analysis of conformation at elevated temperatures

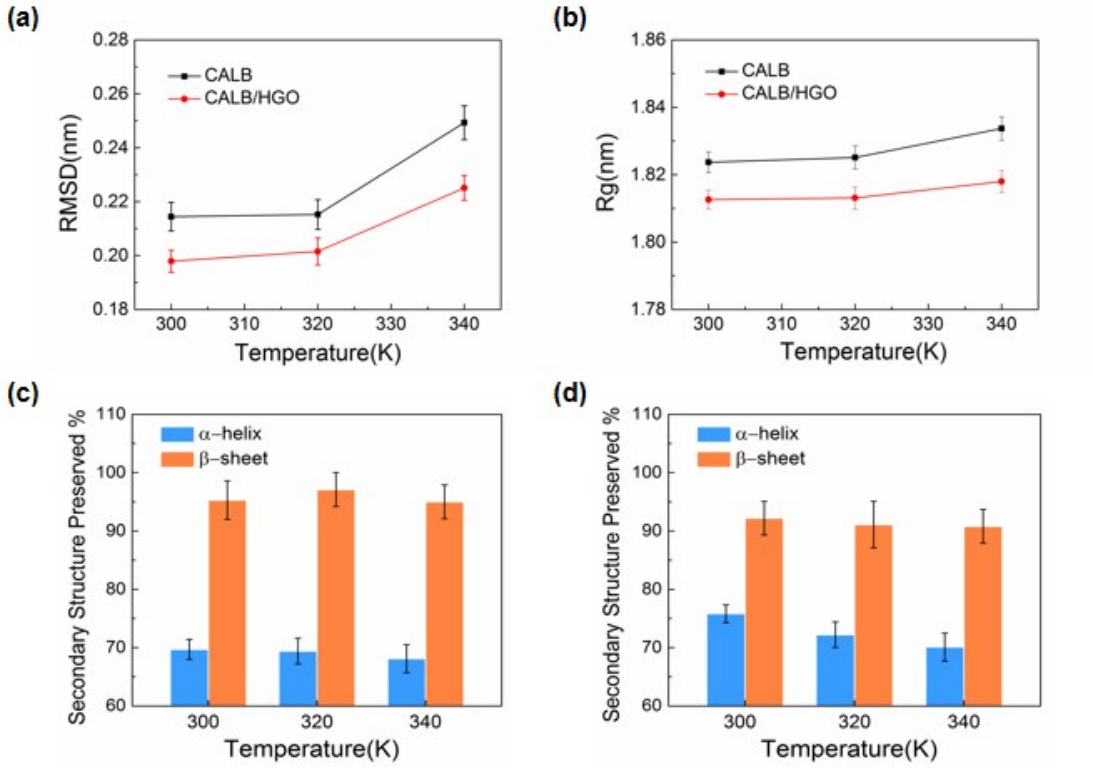

Fig. S3 (a) RMSD of CALB backbone. (b) Rg values of CALB. (c) Preserved secondary structure of CALB. (d) Preserved secondary structure of CALB in CALB/HGO assembly. Results were calculated from the last 1 ns of the simulations.

SI 5. Analysis of B-factors of active region

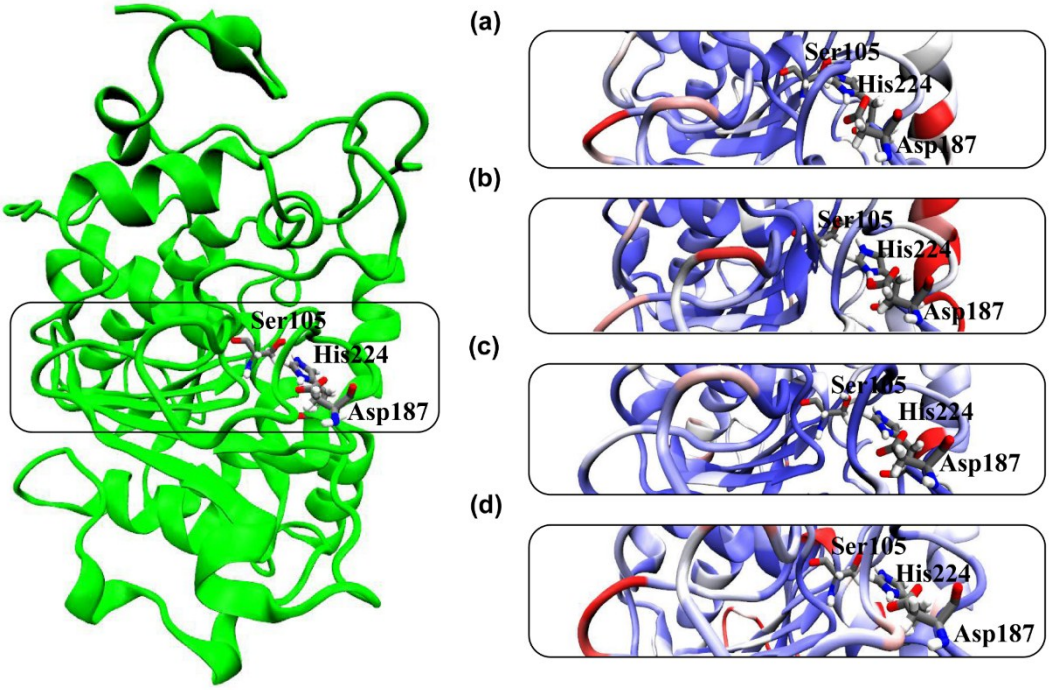

Fig. S4 Flexibility of the active region of CALB as indicated by B-factors: (a) CALB, (b) CALB/GO, (c) CALB/MGO, and (d) CALB/HGO. Blue-white-red colors denote rigid-moderate-flexible regions of the enzyme, respectively.