

## Negative contribution from defects responsible for low Young's modulus of Graphene Oxide at small defect densities

### (Supplementary Information)

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**Contents:** The supporting information contains two tables (Table S1 and Table S2).

**Table S1.** Elemental parameters used in the simulation.

Element	Cov Radius (Å)	Rvdw (Radius of van der Waals) (Å)	Evdw (Energy of van der Waals) (kcal/mol)
C	1.3825	1.9133	0.1853
H	0.7853	1.5904	0.0419
O	1.2477	1.9236	0.0904

**Table S2:** Atom counts at different O/C ratios.

O/C (%)	System	Carbon	Oxygen	Hydrogen
5	dGO	960	9	0
	GO	960	30	1
	rGO	959	5	3
8	dGO	960	9	0
	GO	960	43	1
	rGO	956	8	0
15	dGO	960	34	2
	GO	960	95	3
	rGO	936	29	3
20	dGO	960	55	2
	GO	960	124	5
	rGO	922	53	5

25	<b>dGO</b>	958	59	0
	<b>GO</b>	958	159	11
	<b>rGO</b>	910	56	8

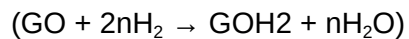
**Table S3:** Contribution of different categories of atoms to the total Young's modulus for 5% and 15% O/C ratios

**5% O/C**

<b>System</b>	<b>D (Gpa)</b>	<b>C<sub>G</sub> (Gpa)</b>	<b>C<sub>O</sub> + O/H</b>	<b>Total Young's modulus (GPa)</b>
<b>Graphene</b>	0.00	526.27	0.0	526.27
<b>Oxidized</b>	0.0	570.73	-65.65	505.08
<b>dGO</b>	19.17	437.60	-6.5	450.27
<b>GO</b>	-12.77	437.30	-13.48	411.05

**15% O/C**

<b>System</b>	<b>D (Gpa)</b>	<b>C<sub>G</sub> (Gpa)</b>	<b>C<sub>O</sub> + O/H</b>	<b>Total Young's modulus (GPa)</b>
<b>Graphene</b>	0.00	526.27	0.0	526.27
<b>Oxidized</b>	0.0	631.91	-125.86	506.05
<b>dGO</b>	42.43	334.60	0.37	377.40
<b>GO</b>	97.92	245.40	-14.03	329.29

**Table S4:** Thermochemistry of substitution of oxygen atoms by hydrogen atoms in graphene oxide

	n = 1	n = 32	n = 32 (averaged over snapshots)
$E_{\text{GO}}$	-190391.81 kcal/mol	-190391.81 kcal/mol	-190657.36 kcal/mol
$2nE_{\text{H}_2}$	2x(-58.78) kcal/mol	64x(-58.78) kcal/mol	64x(-58.78) kcal/mol
$nE_{\text{H}_2\text{O}}$	-235.68 kcal/mol	32x(-235.68) kcal/mol	32x(-235.68) kcal/mol
$E_{\text{GOH}_2}$	-190325.32 kcal/mol	-191020.56 kcal/mol	-191955.01 kcal/mol
$\Delta E$	-51.68 kcal/mol	-4407.72 kcal/mol	-5077.49 kcal/mol
$\Delta E/n$	-51.68 kcal/mol	-137.74 kcal/mol	-158.67 kcal/mol