

Electronic Supplementary Information for

Thermodynamic and Redox Properties of Graphene Oxides for Lithium-Ion Battery Applications: First Principles Density Functional Theory Modeling Approach

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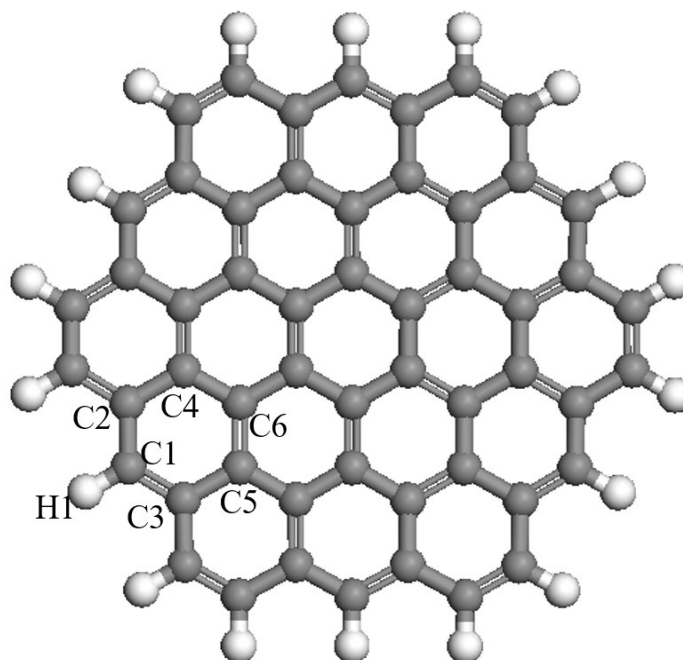
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1. Determination of the atomic charges

All the atomic charges in our study are determined by the Mulliken population analysis combined with the density functional theory (DFT) method at the B3LYP level of theory and 6-31G(d,p) basis set in the Jaguar package. Figures S1-S illustrate the cluster models utilized to calculate the atomic charges and their atomic charges.

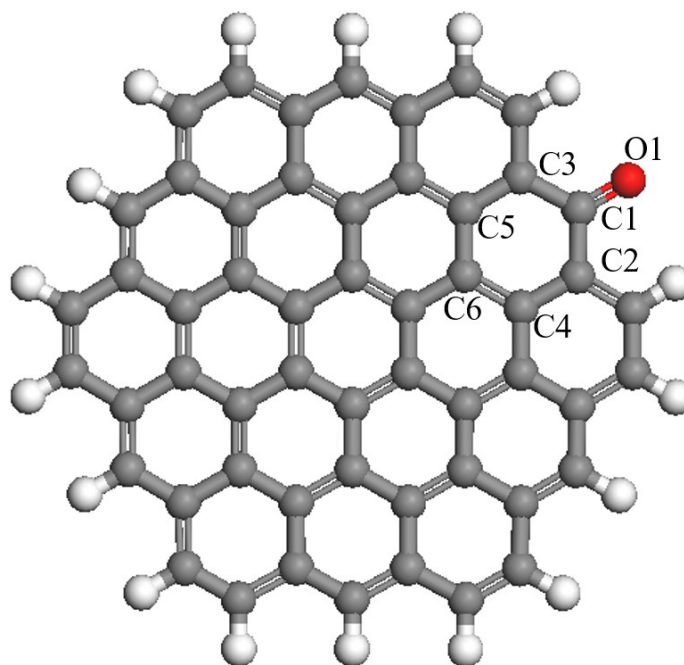
Pristine graphene



Type	Charge
H1	0.16
C1	-0.17
C2	0.04
C3	0.04
C4	-0.04
C5	-0.03
C6	0.005

Figure S1: The atomic charges for the pristine graphene.

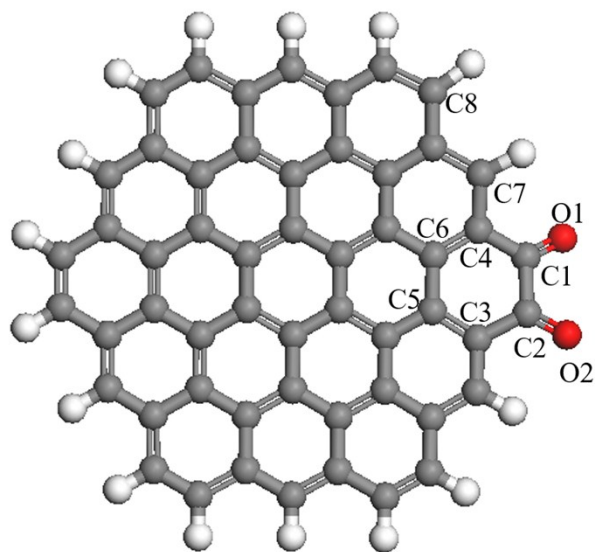
Graphene with 1 carbonyl group



Type	Charge
O1	-0.45
C1	0.33
C2	0.08
C3	0.08
C4	0.004
C5	0.004
C6	0.0004

Figure S2: The atomic charges for the graphene with 1 carbonyl group.

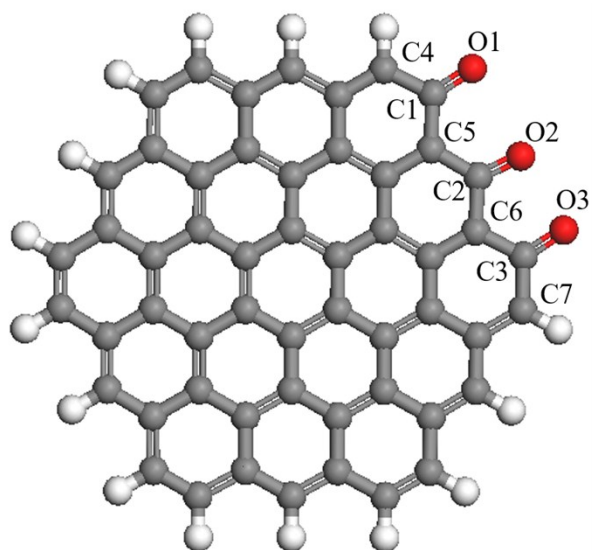
Graphene with 2 locally distributed carbonyl groups



Type	Charge
O1	-0.37
O2	-0.37
C1	-0.17
C2	-0.13
C3	-0.06
C4	0.04
C5	0.004
C6	0.0004
C7	0.32
C8	0.30

Figure S3: The atomic charges for the graphene with 2 locally distributed carbonyl groups.

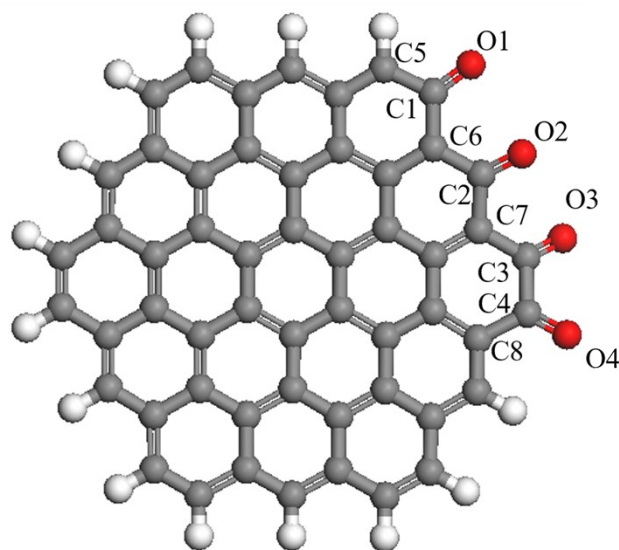
Graphene with 3 locally distributed carbonyl groups



Type	Charge
O1	-0.45
O2	-0.21
O3	-0.36
C1	0.33
C2	0.30
C3	0.31
C4	-0.21
C5	-0.16
C6	-0.15
C7	-0.22

Figure S4: The atomic charges for the graphene with 3 locally distributed carbonyl groups.

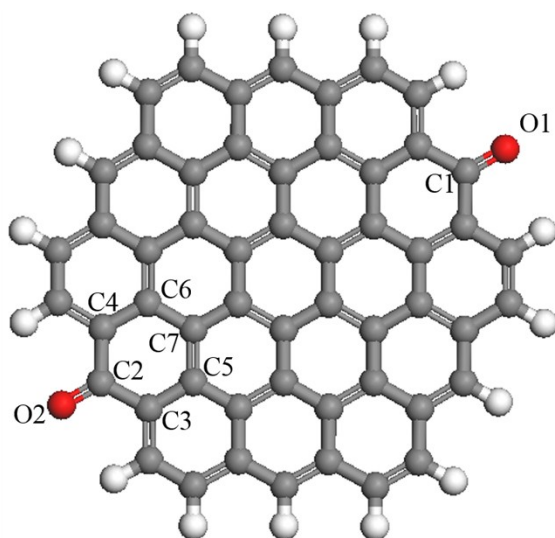
Graphene with 4 locally distributed carbonyl groups



Type	Charge
O1	-0.42
O2	-0.35
O3	-0.31
O4	-0.37
C1	0.32
C2	0.33
C3	0.25
C4	0.29
C5	-0.17
C6	-0.14
C7	-0.08
C8	-0.04

Figure S5: The atomic charges for the graphene with 4 locally distributed carbonyl groups.

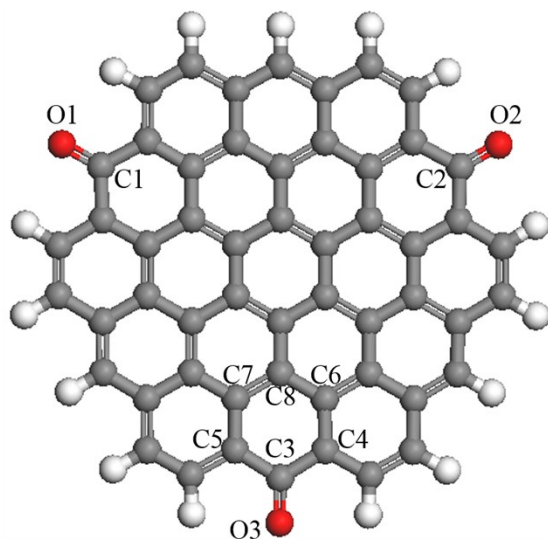
Graphene with 2 uniformly distributed carbonyl groups



Type	Charge
O1	-0.42
O2	-0.42
C1	0.33
C2	0.33
C3	-0.07
C4	-0.08
C5	0.004
C6	0.004
C7	0.02

Figure S6: The atomic charges for the graphene with 2 uniformly distributed carbonyl groups.

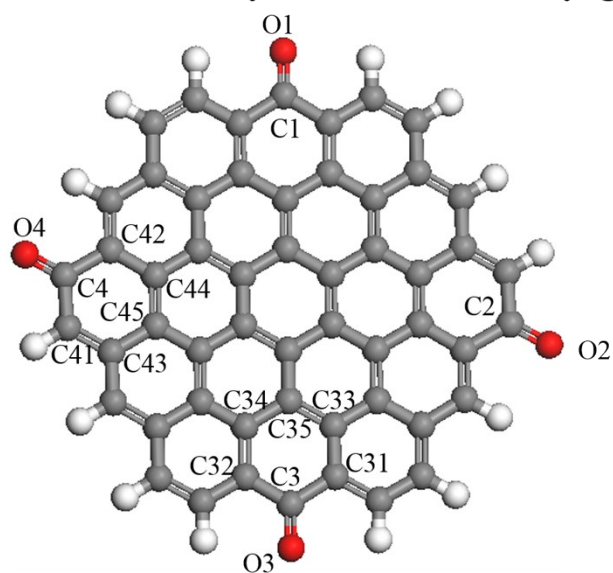
Graphene with 3 uniformly distributed carbonyl groups



Type	Charge
O1	-0.44
O2	-0.47
O3	-0.46
C1	0.34
C2	0.33
C3	0.33
C4	-0.06
C5	-0.06
C6	-0.005
C7	-0.006
C8	0.03

Figure S7: The atomic charges for the graphene with 3 uniformly distributed carbonyl groups.

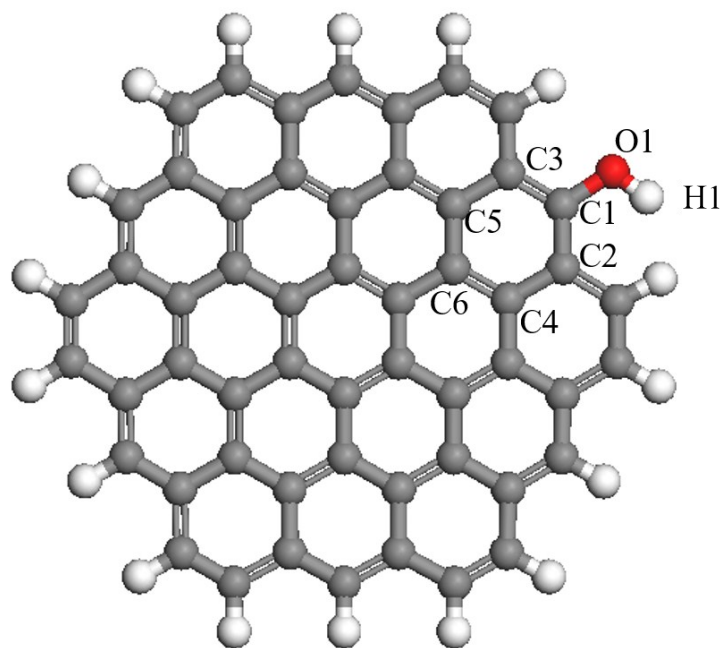
Graphene with 4 uniformly distributed carbonyl groups



Type	Charge	Type	Charge
O1	-0.41	C31	-0.07
O2	-0.44	C32	-0.07
O3	-0.41	C33	0.0005
O4	-0.44	C34	-0.01
C1	0.32	C35	0.02
C2	0.32	C41	-0.20
C3	0.32	C42	-0.06
C4	0.32	C43	0.07
		C44	0.01
		C45	-0.009

Figure S8: The atomic charges for the graphene with 4 uniformly distributed carbonyl groups.

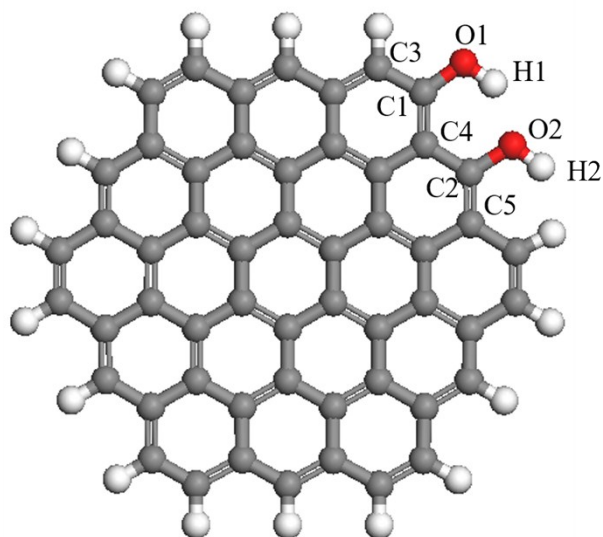
Graphene with 1 hydroxyl group



Type	Charge
O1	-0.47
H1	0.36
C1	0.26
C2	-0.02
C3	-0.07
C4	0.002
C5	0.005
C6	-0.002

Figure S9: The atomic charges for the graphene with 1 hydroxyl group.

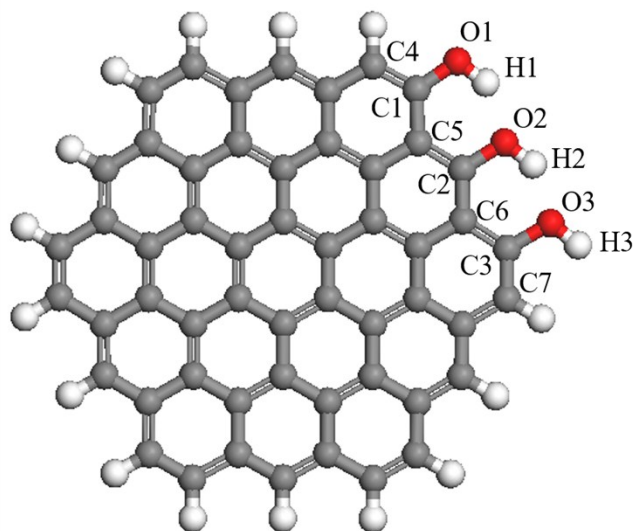
Graphene with 2 locally distributed hydroxyl groups



Type	Charge
O1	-0.58
O2	-0.57
H1	0.46
H2	0.43
C1	0.28
C2	0.26
C3	-0.29
C4	-0.14
C5	-0.03

Figure S10: The atomic charges for the graphene with 2 locally distributed hydroxyl groups.

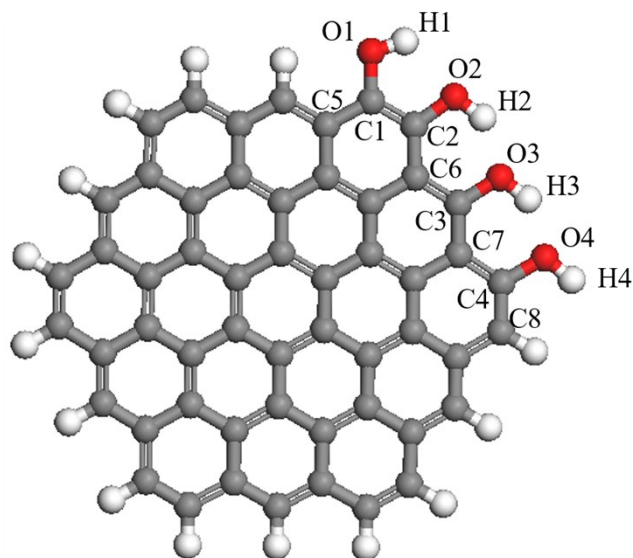
Graphene with 3 locally distributed hydroxyl groups



Type	Charge
O1	-0.52
O2	-0.63
O3	-0.61
H1	0.43
H2	0.46
H3	0.41
C1	0.27
C2	0.27
C3	0.30
C4	-0.26
C5	-0.13
C6	-0.12
C7	-0.27

Figure S11: The atomic charges for the graphene with 3 locally distributed hydroxyl groups.

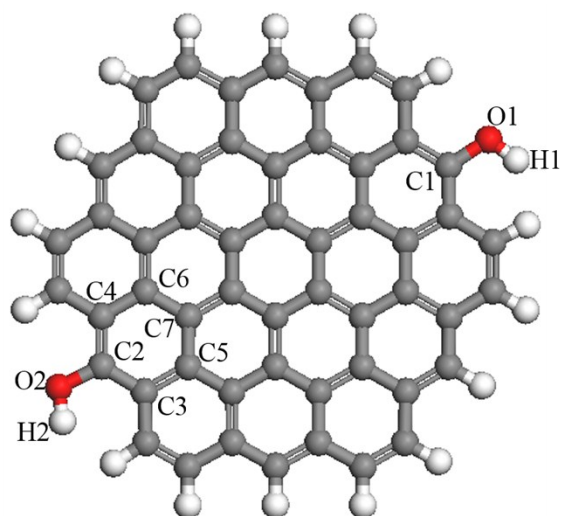
Graphene with 4 locally distributed hydroxyl groups



Type	Charge
O1	-0.51
O2	-0.60
O3	-0.63
O4	-0.60
H1	0.41
H2	0.45
H3	0.46
H4	0.41
C1	0.17
C2	0.17
C3	0.26
C4	0.29
C5	-0.02
C6	-0.09
C7	-0.14
C8	-0.26

Figure S12: The atomic charges for the graphene with 4 locally distributed hydroxyl groups.

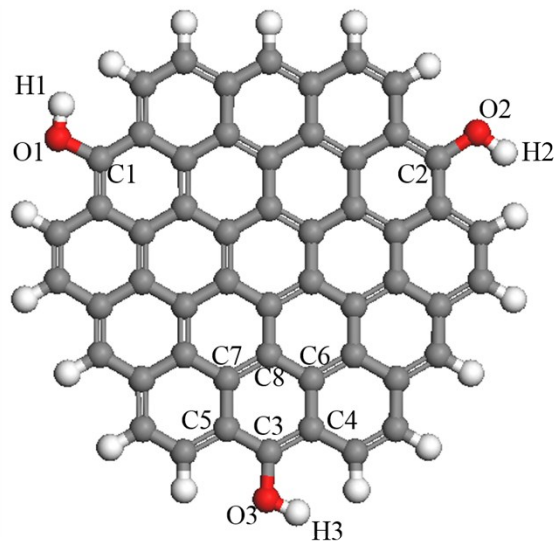
Graphene with 2 uniformly distributed hydroxyl groups



Type	Charge
O1	-0.45
O2	-0.45
H1	0.36
H2	0.36
C1	0.23
C2	0.23
C3	-0.02
C4	-0.08
C5	0.005
C6	0.008
C7	0.01

Figure S13: The atomic charges for the graphene with 2 uniformly distributed hydroxyl groups.

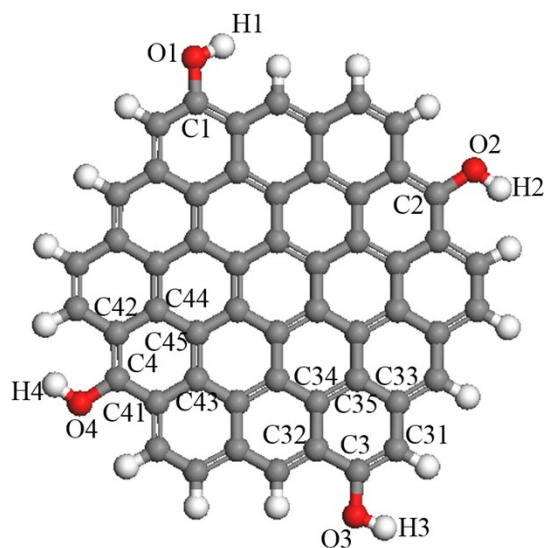
Graphene with 3 uniformly distributed hydroxyl groups



Type	Charge
O1	-0.46
O2	-0.46
O3	-0.46
H1	0.36
H2	0.36
H3	0.36
C1	0.25
C2	0.25
C3	0.25
C4	-0.01
C5	-0.07
C6	-0.0007
C7	0.003
C8	0.008

Figure S14: The atomic charges for the graphene with 3 uniformly distributed hydroxyl groups.

Graphene with 4 uniformly distributed hydroxyl groups



Type	Charge	Type	Charge
O1	-0.47	C31	-0.27
O2	-0.45	C32	-0.06
O3	-0.50	C33	0.08
O4	-0.45	C34	0.02
H1	0.35	C35	-0.03
H2	0.36	C41	-0.07
H3	0.37	C42	-0.01
H4	0.36	C43	0.001
C1	0.25	C44	0.004
C2	0.24	C45	0.003
C3	0.28		
C4	0.24		

Figure S15: The atomic charges for the graphene with 4 uniformly distributed hydroxyl groups.