Supporting Information for

Distribution of Oxygen-Containing Functional Groups on Defective Graphene: Properties Engineering and Li Adsorption

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Keywords: First-principles calculations; Defects; Oxygen-containing functional groups; 2D carbon materials; Lithium storage.

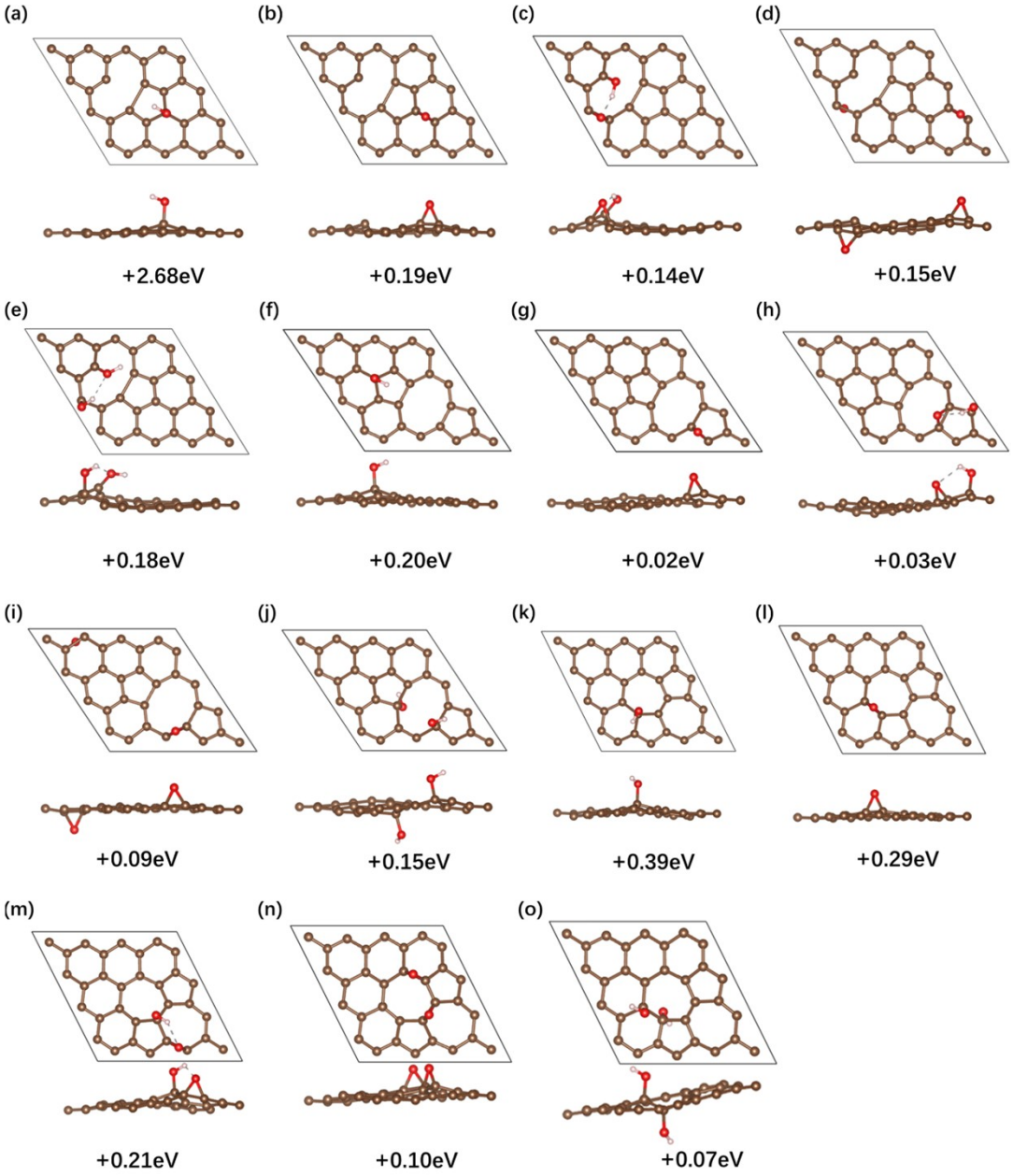

Figure S1. The second stable structures of multi-defect GOs. (a)-(o) are SV-OH-2, SV-O-2, SV-O&OH-2, SV-O&O-2, SV-OH&OH-2, DV-OH-2, DV-O-2, DV-O&OH-2, DV-O&O-2, DV-OH&OH-2, SW-OH-2, SW-O-2, SW-O&OH-2, SW-O&O-2, SW-OH&OH-2.

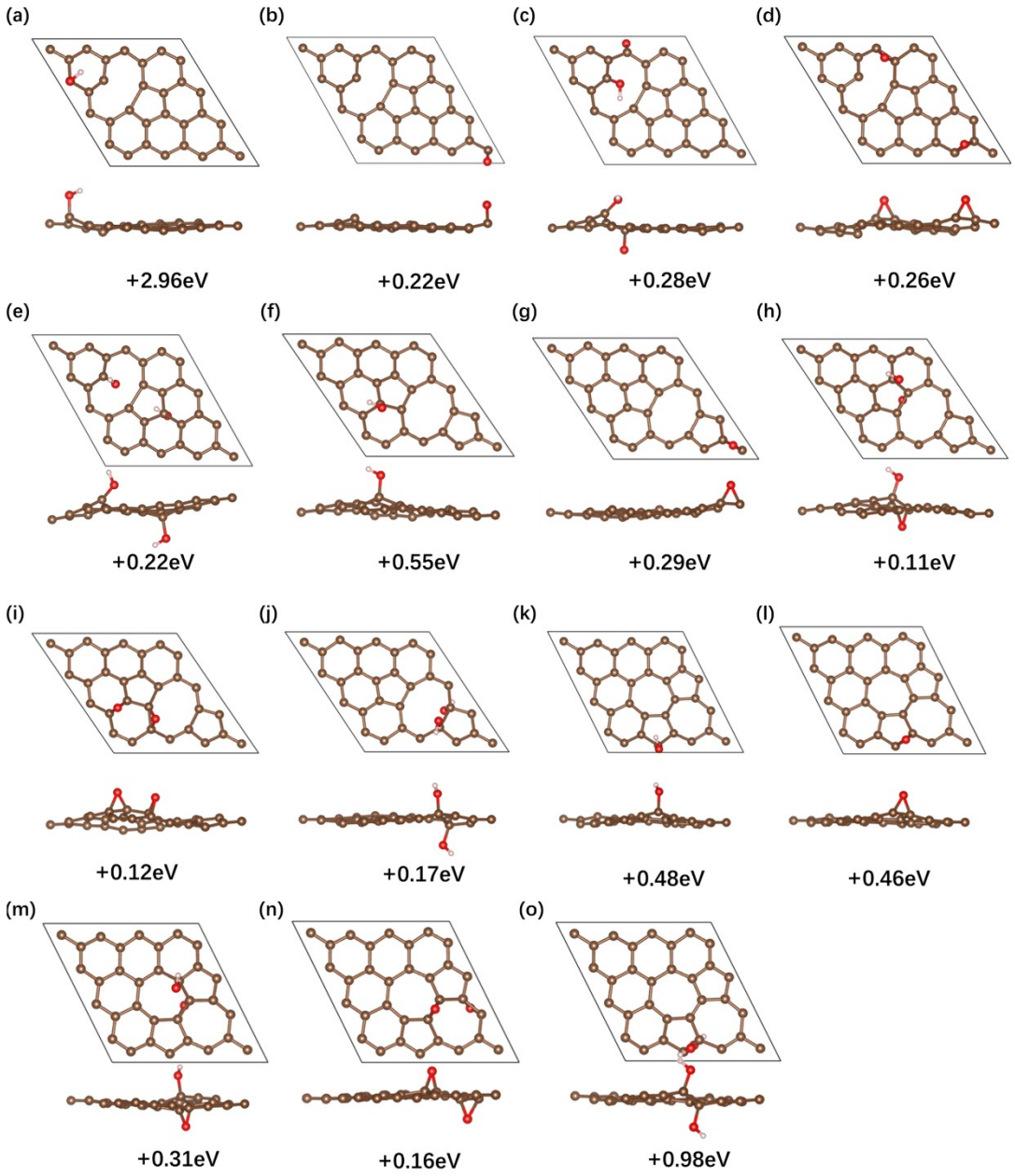

Figure S2. The third stable structures of multi-defect GOs. (a)-(o) are SV-OH-3, SV-O-3, SV-O&OH-3, SV-O&O-3, SV-OH&OH-3, DV-OH-3, DV-O-3, DV-O&OH-3, DV-O&O-3, DV-OH&OH-3, SW-OH-3, SW-O-3, SW-O&OH-3, SW-O&O-3, SW-OH&OH-3.

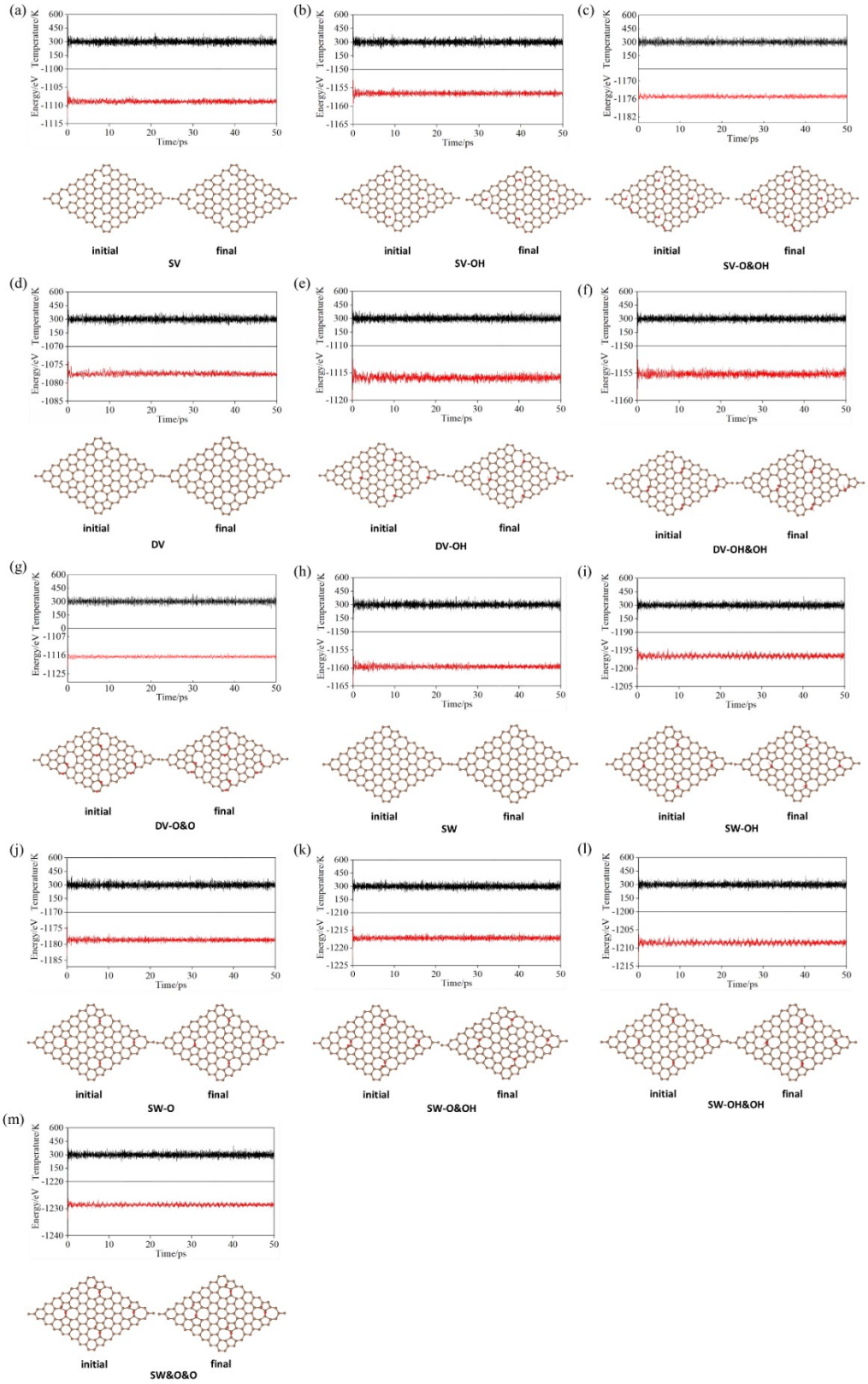

Figure S3. The energy and temperature variations for AIMD simulations of (a) SV, (b) SV-OH, (c) SV-O&OH, (d) DV, (e) DV-OH, (f) DV-OH&OH, (g) DV-O&O, (h) SW, (i) SW-OH, (j) SW-O, (k) SW-O&OH, (l) SW-OH&OH, (m) SW-O&O. The inset illustrates the top view of the structures before and after the 50 ps AIMD simulations.

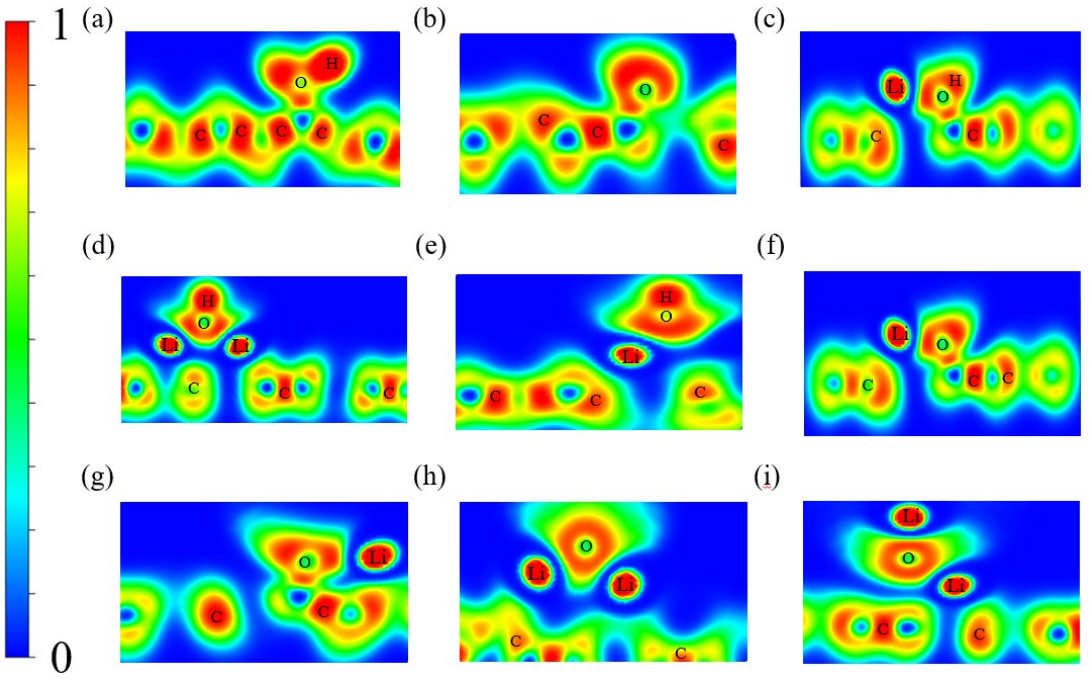

Figure S4. Electron localization functions for (a) DV-OH, (b) DV-O, (c) DV-LiOH, (d) DV-Li_2OH, (e) DV-Li_3OH, (f) DV-LiO, (g) DV-Li_2O, (h) DV- Li_3O (i) DV-Li_4O.

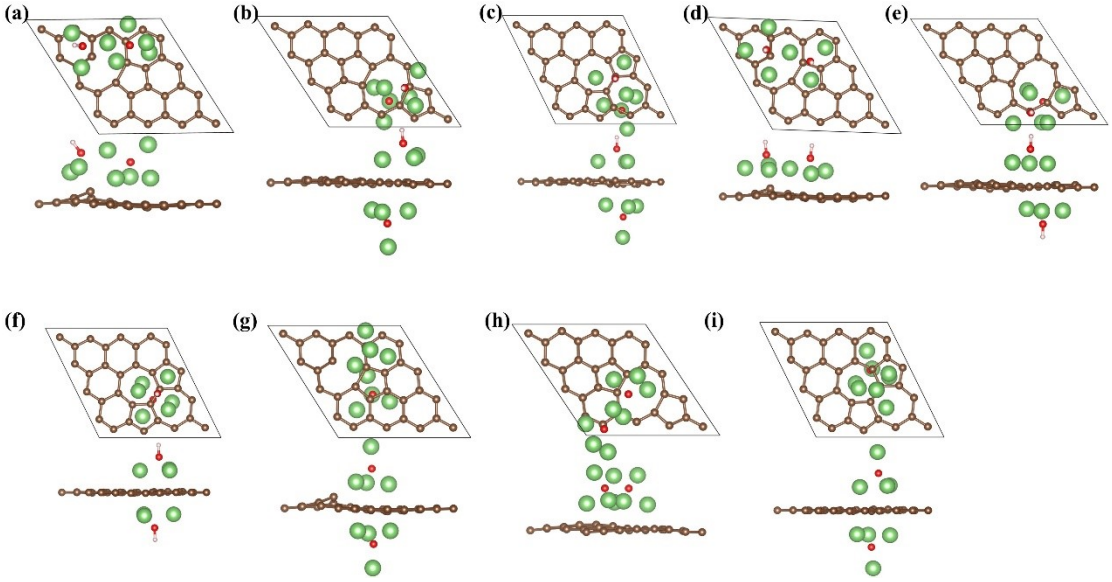

Figure S5. Optimized configurations for the absorption of Li atoms on graphene with SV (a, d, g), DV (b, e, h), and SW (c, f, i) containing two oxygen-containing functional groups.

Table S1. The table lists the formation energy (E_f) for all stable configurations. The

Structure	E_f	Structure	E_f
SV	0.18	SV-Li_2OH	-0.49
SV-OH	-0.44	SV-Li_3OH	-0.50
SV-O	-0.11	SV-LiO	-0.18
SV-O&OH	-0.71	SV-Li_2O	-0.23
SV-O&O	-0.40	SV-Li_3O	-0.26
SV-OH&OH	-0.94	SV-Li_4O	-0.28
SV-Li	0.11	SV-Li_4O-Li_3OH	-0.78
SV-7Li	0.14	SV-2*Li_4O	-0.56
SV-LiOH	-0.48	SV-2*Li_3OH	-0.93
DV	0.14	DV-Li_2OH	-0.52
DV-OH	-0.43	DV-Li_3OH	-0.50
DV-O	-0.18	DV-LiO	-0.25
DV-O&OH	-0.72	DV-Li_2O	-0.29
DV-O&O	-0.48	DV-Li_3O	-0.32
DV-OH&OH	-0.96	DV-Li_4O	-0.34
DV-Li	0.10	DV-Li_4O-Li_3OH	-0.69
DV-5Li	0.12	DV-2*Li_4O	-0.67
DV-LiOH	-0.48	DV-2*Li_3OH	-0.99
SW	0.06	SW-Li_2OH	-0.54
SW-OH	-0.46	SW-Li_3OH	-0.56
SW-O	-0.24	SW-LiO	-0.26
SW-O&OH	-0.74	SW-Li_2O	-0.32
SW-O&O	-0.52	SW-Li_3O	-0.35
SW-OH&OH	-0.96	SW-Li_4O	-0.36
SW-Li	0.04	SW-Li_4O-Li_3OH	-0.82
SW-4Li	0.05	SW-2*Li_4O	-0.65
SW-LiOH	-0.51	SW-2*Li_3OH	-0.99

formation energy is given in eV/atom.