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

Supplementary Information

for

Gas adsorption efficacy of Graphene sheet Functionalised with Carboxyl, Hydroxyl and Epoxy groups in conjunction with Stone-Thrower wales (STW) and Inverse Stone-Thrower Wales (ISTW) defect

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Adsorption on single-side functionalised sheets:

Table S1: Optimized C-C bond length in functionalised pristine and defective sheets.

	Single side functionalization							
	Central C-C bond length (Å)	**C-C-C bond angle (º)**		**Central C-C bond length (Å)**	**C-C-C bond angle (º)**		**C-C bond length (Å)**	**C-C-C bond angle (º)**
Pristine	1.39	120	STW	1.33	125.5	ISTW	1.36	109.2
Pris.+COOH	1.51	112.7	STW+COOH	1.46	114.5	ISTW+COOH	1.53	101.8
Pris.+OH	1.50	112.7	STW+OH	1.46	114.0	ISTW+OH	1.53	101.8
Pris.+ C-O-C	1.49	118.2	STW+ C-O-C	1.44	123.7	ISTW+ C-O-C	1.47	106.9

Table S2: Mulliken Charges accumulated on the gas molecule in the adsorbed complexes.

Complex	Mulliken charges on gas molecule (e)						
	CO_2	H_2	N_2	CH_4	HF	O_2	H_2O
Pristine sheet	0.0118	0.0044	0.0029	0.0101	0.0127	-0.0515	0.0170
Pristine+COOH	0.0046	-0.0067	0.0149	-0.0169	-0.0163	0.0155	0.0402
Pristine+OH	-0.0051	-0.0153	0.0058	-0.0068	-0.0314	-0.2927	-0.0168
Pristine+ C-O-C	-0.0011	-0.0102	0.0020	-0.0075	-0.0250	0.0122	-0.0058
STW sheet	0.0115	0.0029	0.0031	0.0084	0.0076	-0.0677	0.0184
STW+COOH	0.0042	-0.0065	0.0146	-0.0157	-0.0162	0.0154	0.0396
STW+OH	-0.0030	-0.0209	0.0009	0.0057	0.0378	0.0137	0.0672
STW+ C-O-C	-0.0037	-0.0156	0.0013	-0.0094	-0.0238	0.0110	-0.0092
ISTW sheet	0.0075	-0.0018	-0.0584	0.0029	0.0005	-0.1628	0.0120
ISTW+COOH	0.0042	-0.0076	0.0147	-0.0172	-0.0169	0.0107	0.0382
ISTW+OH	-0.0050	-0.0205	0.0001	-0.0162	-0.0281	0.0115	0.0677
ISTW+ C-O-C	-0.0008	-0.0118	0.0031	-0.0005	-0.0277	0.0069	-0.0051

Table S3: Adsorptivity of the defect

Gas	Adsorptivity of the defect					
	STW Def-Perfect (COOH)	**STW Def-Perfect(OH)**	**STW Def-Perfect (C-O-C)**	**STW Def/Perf (COOH)**	**STW Def/Perf (OH)**	**STW Def/Perf (C-O-C)**
CO_2	0.002	0.002	0.011	0.992	0.993	0.957
H_2	-0.001	0.008	0.001	1.014	0.929	0.989
N_2	0	0.036	0	1	0.808	1
CH_4	0	0.022	0.006	1	0.907	0.972
HF	-0.001	0.183	0.015	1.001	0.687	0.971
O_2	0	-1.188	0.017	1	2.833	0.900
H_2O	0	-0.117	0.011	1	1.269	0.971
	ISTW Def-Perfect (COOH)	**ISTW Def-Perfect(OH)**	**ISTW Def-Perfect (C-O-C)**	**ISTW Def/Perf (COOH)**	**ISTW Def/Perf (OH)**	**ISTW Def/Perf (C-O-C)**
CO_2	0.006	0.018	0.029	0.977	0.937	0.887
H_2	0.001	0.019	0.012	0.985	0.833	0.875
N_2	0.005	0.037	0.009	0.958	0.803	0.933
CH_4	0.003	0.042	0.032	0.975	0.824	0.851
HF	0	0.043	0.028	1	0.926	0.945
O_2	1.589	-1.182	0.027	0.105	2.824	0.842
H_2O	0.008	-0.111	0.027	0.987	1.255	0.928

Table S4: Optimized C-C bond length and C-C-C bond angle in bi-functionalised defective sheets.

	Bi-functionalization						
		Central C-C bond length (C-O) (Å)	**C-C-C bond angle (º)**			**Central C-C bond length (Å)**	**C-C-C bond angle (º)**
STW	-	1.33	125.56	ISTW	-	1.36	109.27
STW+2COOH	Above	1.52	118.39	ISTW+2COOH	Above	1.59	103.45
	Below	1.52	112.61		Below	1.51	103.78, 98.47
STW+2OH	Above	1.53	118.38	ISTW+2OH	Above	1.58	104.38,103.86
	Below	1.50	111.74		Below	1.53	103.70, 97.23
STW+2C-O-C	Above	1.48	121.15	ISTW+2C-O-C	Above	1.47	105.22, 108.42
	Below	1.85(1.40)	-		Below	1.81(1.41)	-

Table S5: Energy Decomposition Analysis performed for N_2/ISTW sheet using BHand HLYP/TZP with dispersion correction as implemented in Amsterdam Density Functional theory (ADF) package

rGO	Energy components (in eV)				
	ΔE_{elstat}	ΔE_{pauli}	$\Delta E_{orb.}$	$\Delta E_{disp.}$	ΔE_{int}
N_2/ISTW	-12.21	33.47	-21.62	-0.22	-0.57