Supporting Information

Mechanistic Study of Graphitic Carbon Layer and Nanospheres Formation on the Surface of T-ZnO

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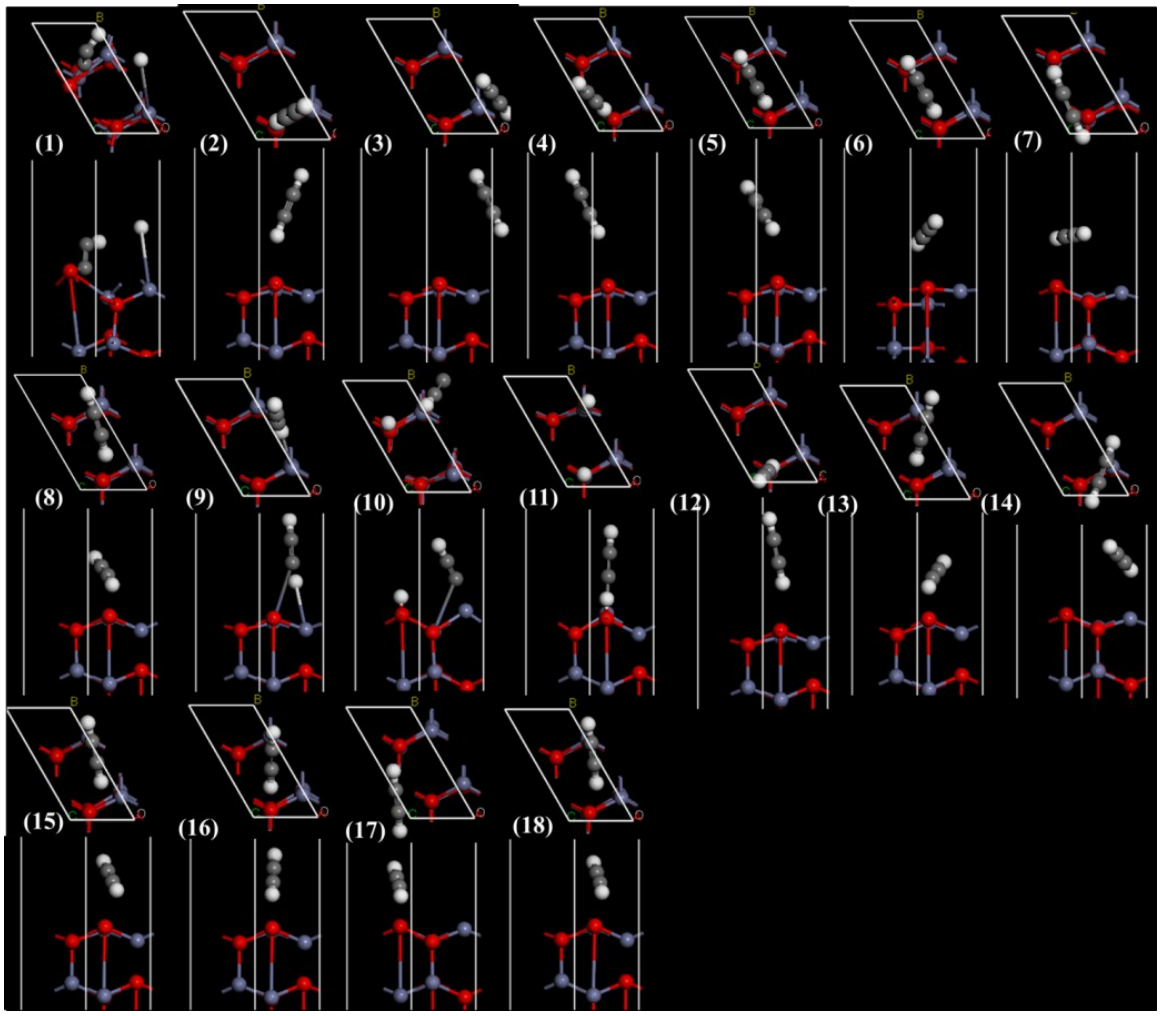

Figure S1. Calculated structures of absorption on (001) ZnO surface.

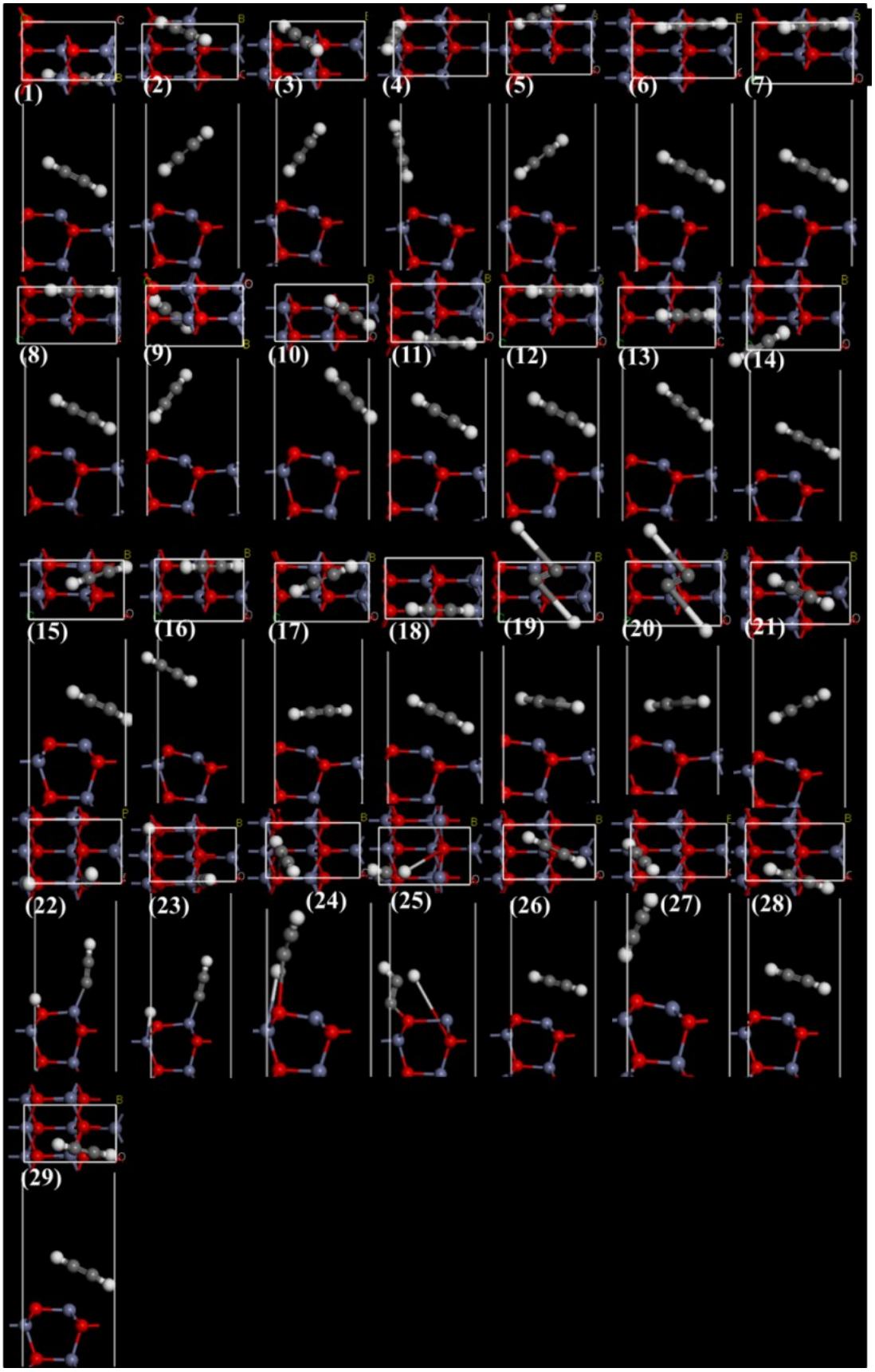

Figure S2. Calculated structures of absorption on (100) ZnO surface.

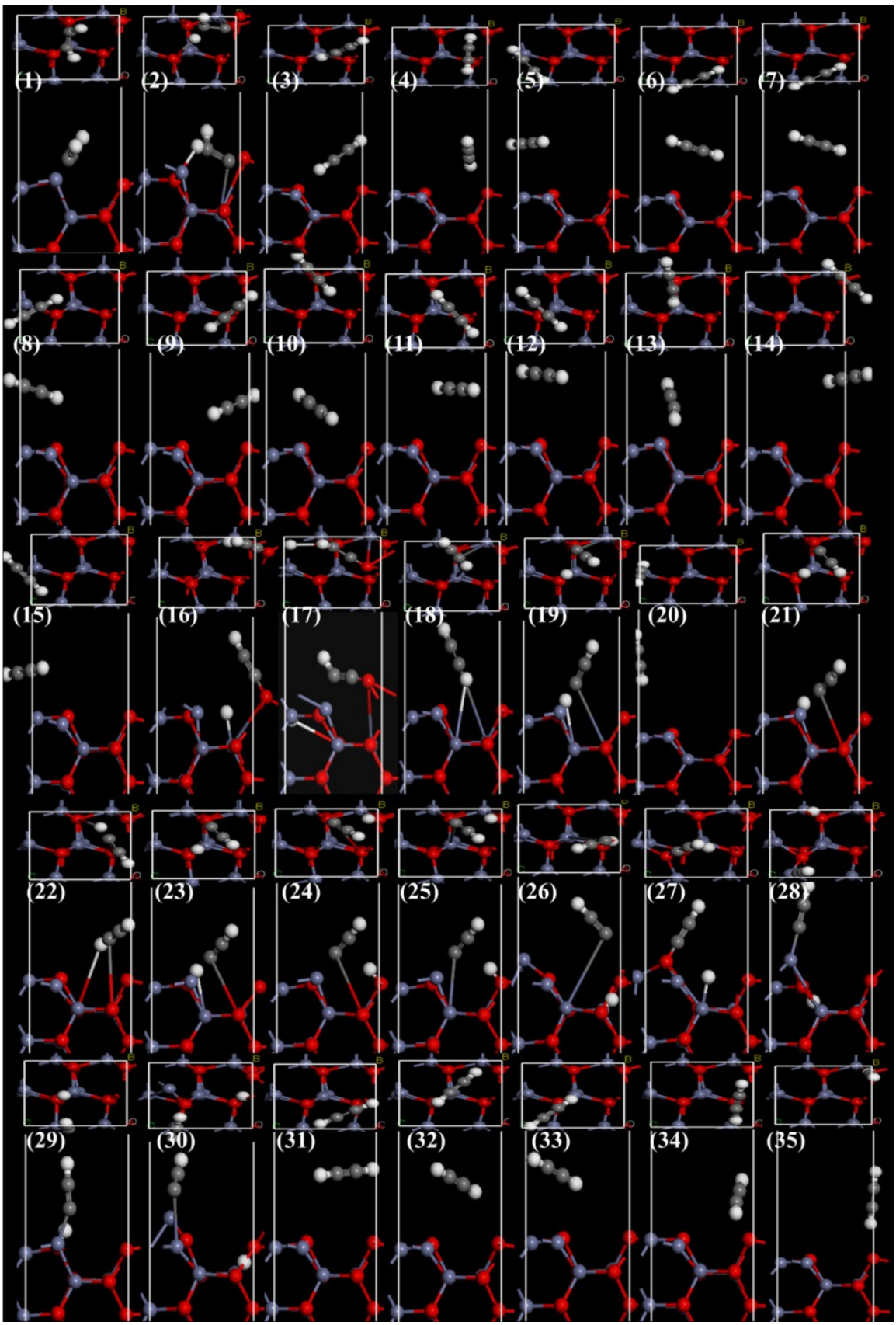

Figure S3. Calculated structures of absorption on (110) ZnO surface (part A).

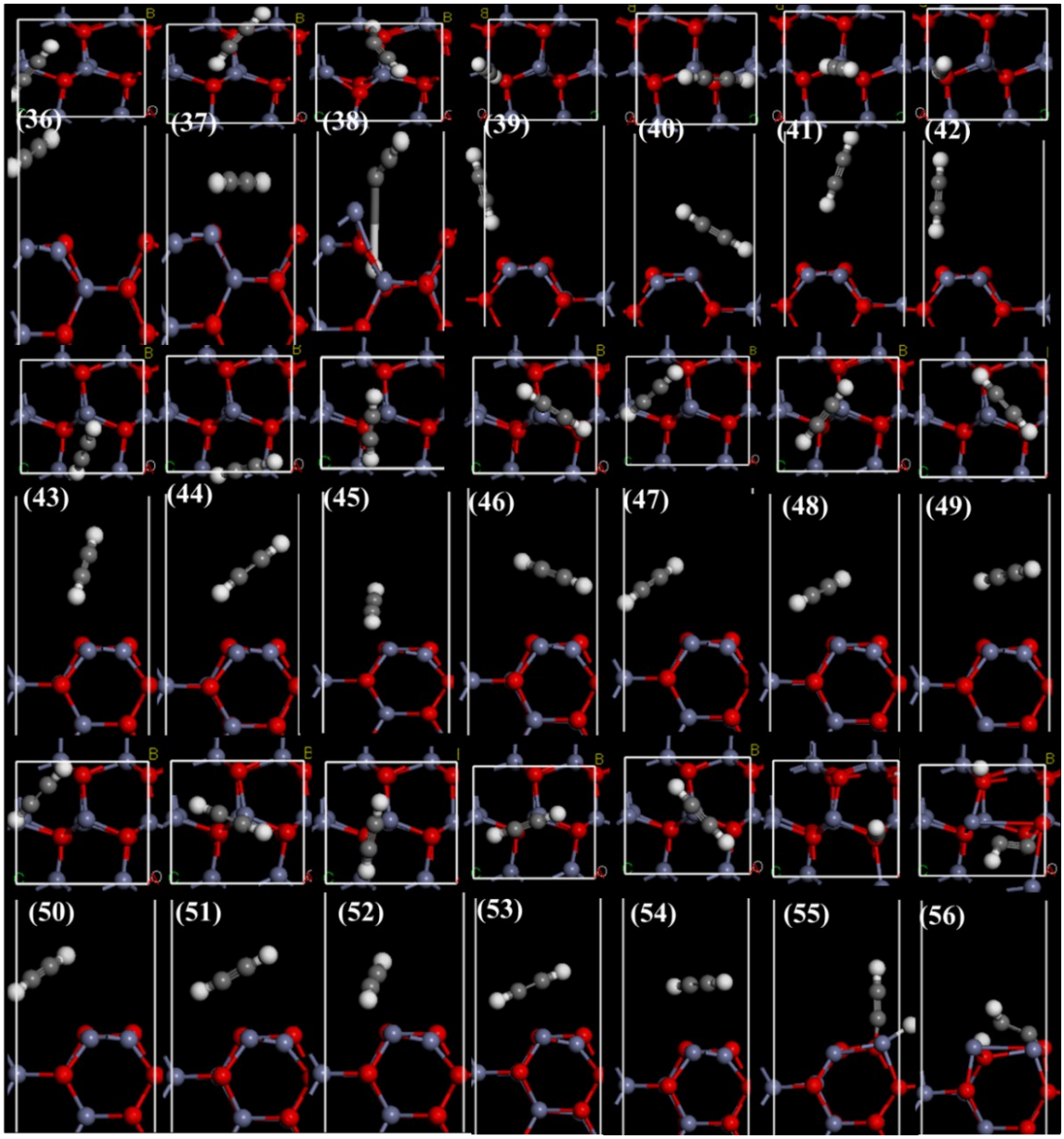

Figure S4. Calculated structures of absorption on (110) ZnO surface (part B).

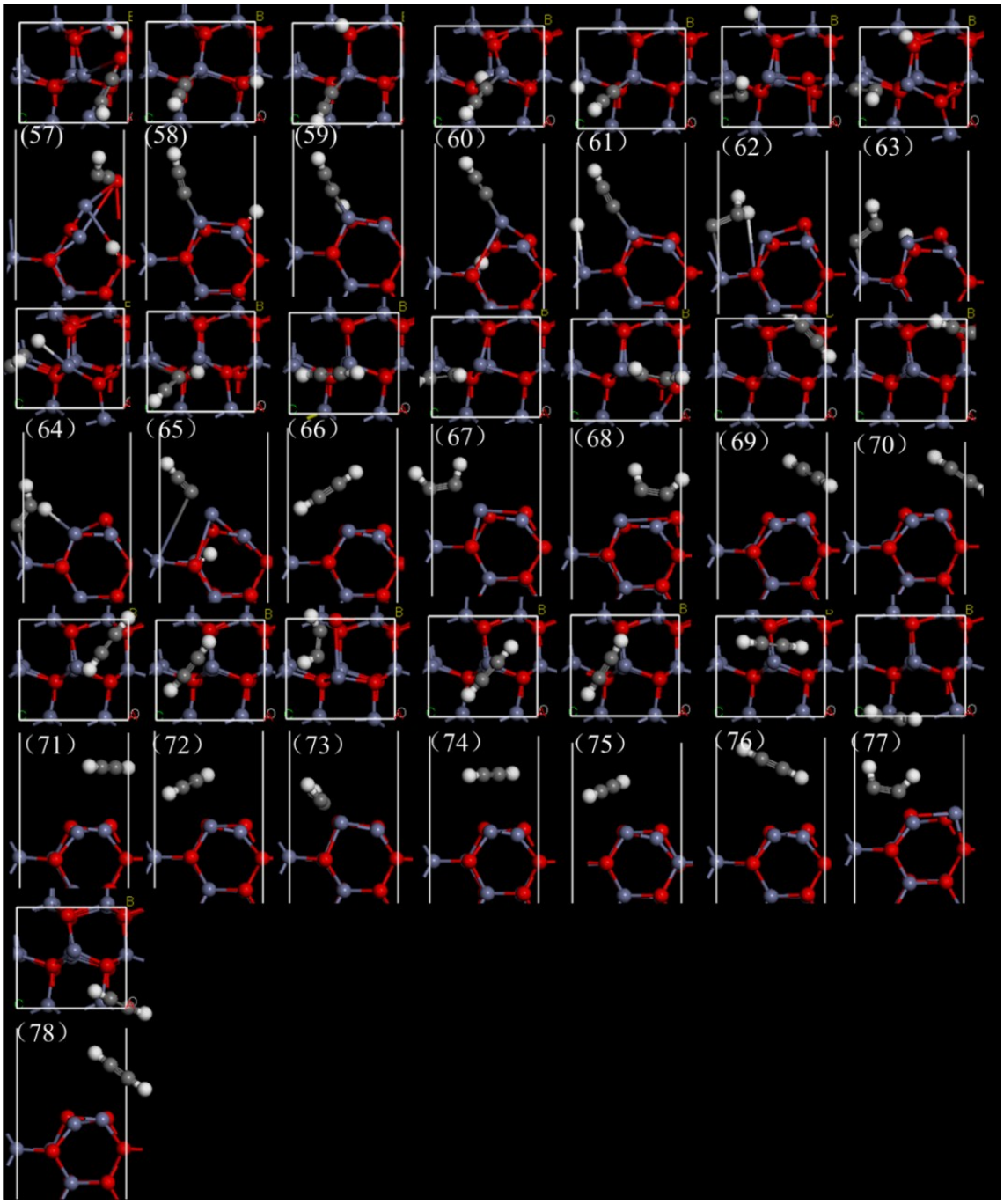

Figure S5. Calculated structures of absorption on (110) ZnO surface (part C).

Table S1. Calculated parameters for structure on (0 0 1) surface*.

absorbate	structure	BE (ev)	∠HCC (°)	∠CCH (°)	d(H-C) (Å)	d(C-C) (Å)	d(C-H) (Å)	d(ads-sub) (Å)	d⊥(ads-sub)(Å)
Free C_2H_2	Calc.		180	180	1.086	1.206	1.086		
C_2H_2/ZnO (0 0 1)	1	-1.06		118.9	1.095	1.323	1.089	1.420	1.363
	2	-0.42	179.2	178.3	1.071	1.206	1.066	2.444	2.427
	3	-0.42	178.9	178.8	1.067	1.206	1.065	3.632	2.707
	4	-0.42	178.3	177.9	1.068	1.205	1.066	2.81	2.718
	5	-0.45	178.4	177.5	1.07	1.205	1.068	2.838	2.702
	6	-0.30	179.1	179.3	1.069	1.205	1.068	3.014	2.180
	7	-0.48	177.6	178.8	1.068	1.208	1.067	2.516	2.415
	8	-0.59	174.1	176.4	1.093	1.215	1.077	2.051	1.586
	9	-0.13		176.3	1.086	1.246	1.081	2.662	1.856
	10	-0.60		174.8	3.635	1.224	1.069	0.996	0.717
	11	-0.55		178.7	3.633	1.22	1.069	0.987	0.739
	12	-0.40	178.6	179.2	1.075	1.207	1.07	2.391	2.693
	13	-0.27		121.4	3.543	1.34	1.085	1.377	0.167
	14	-0.63	174.4	177.4	1.086	1.214	1.072	2.062	1.594
	15	-0.49	178.1	179.2	1.073	1.208	1.068	2.731	2.245
	16	-0.55	177.9	178.7	1.077	1.209	1.07	2.48	1.853
	17	-0.57	179.1	177.4	1.085	1.211	1.07	2.071	1.698
	18	-0.65	175.9	177.6	1.088	1.214	1.072	3.173	1.670
	19	-0.58	179.1	177.4	1.085	1.211	1.07	2.071	1.695

* Parameters: BE, binding energy; ∠HCC, the angle of HCC in acetylene; ∠HCC, the angle of CCH in acetylene; d(ads-sub), shortest adsorbate-substrate distance; d⊥(ads-sub), shortest perpendicular height of bent or discomposed acetylene above the top ZnO surface layer.

Table S2. Calculated parameters for structure on (1 0 0) surface*.

absorbate	structure	BE (eV)	∠HCC(°)	∠CCH(°)	d(H-C) (Å)	d(C-C) (Å)	d(C-H) (Å)	d(ads-sub) (Å)	d⊥(ads-sub)(Å)
Free C_2H_2	Calc.		180	180	1.086	1.206	1.086		
C_2H_2/ZnO(1 0 0)	1	-0.71	174.5	177.5	1.120	1.216	1.069	2.666	1.335
	2	-0.34	178.2	179.2	1.063	1.211	1.069	3.59	2.237
	3	-0.26	177.4	179.1	1.071	1.213	1.07	3.403	2.095
	4	-0.16	178.9	178.9	1.065	1.205	1.067	4.89	4.282
	5	-0.31	179.4	178.8	1.075	1.207	1.065	4.111	2.172
	6	-0.31	177.8	178.5	1.075	1.209	1.069	3.968	2.249
	7	-0.33	179.4	178.9	1.084	1.208	1.076	2.931	2.054
	8	-0.53	174.4	177.7	1.116	1.216	1.07	2.673	1.347
	9	-0.32	178.7	177.9	1.071	1.209	1.607	2.274	2.179
	10	-0.36	177.2	178.4	1.082	1.221	1.065	3.241	1.871
	11	-0.30	175.7	178.3	1.119	1.215	1.069	2.817	1.319
	12	-0.69	174.3	177.4	1.119	1.216	1.069	2.38	1.338
	13	-0.70	174.5	177.6	1.118	1.216	1.069	2.387	1.348
	14	-0.69	178.9	179.7	1.067	1.216	1.067	5.25	4.244
	15	-0.32	171.3	177.2	1.125	1.218	1.069	2.389	1.313
	16	-0.66	174.6	177.5	1.119	1.216	1.069	2.379	1.339
	17	-0.46	179.4	176.2	1.079	1.219	1.081	2.519	2.007
	18	-0.69	174.4	177.4	1.119	1.216	1.069	2.378	1.336
	19	-0.36	71.2	71.2	3.166	1.221	3.159	2.457	1.854
	20	-0.47	72.6	72.7	3.047	1.21	3.102	2.586	2.040
	21	-0.07	179.1	178.1	1.607	1.211	1.065	3.076	2.333
	22	-0.55	112.4	176.8	3.452	1.232	1.073	1	0.740
	23	-0.55		177.6	4.594	1.221	1.076	1	0.714
	24	-0.55		177.9	1.071	1.208	1.066	2.306	2.053
	25	-0.62		119.8	2.125	1.326	1.088	1.473	0.972
	26	-0.19	177.2	178.3	1.074	1.212	1.068	2.909	1.816
	27	-0.28	172.8	177.6	1.09	1.219	1.065	2.43	1.599
	28	-0.39	173.7	177.9	1.116	1.217	1.069	2.388	1.359
	29	-0.11	124.5	113.6	1.091	1.351	1.094	1.407	1.198

* Parameters: BE, binding energy; ∠HCC, the angle of HCC in acetylene; ∠HCC, the angle of CCH in acetylene; d(ads-sub), shortest adsorbate-substrate distance;

$d_{\perp}$(ads-sub), shortest perpendicular height of bent or discomposed acetylene above the top ZnO surface layer.

Table S3. Calculated parameters for structure on (1 1 0) structure*.

absorbate	structure	BE (eV)	∠HCC (°)	∠CCH (°)	d(H-C) (Å)	d(C-C) (Å)	d(C-H) (Å)	d(ads-sub) (Å)	⊥(ads-sub) (Å)
Free C_2H_2	Calc.		180	180	1.086	1.206	1.086		
	1	-1.15	125.7	115.4	1.096	1.332	1.092	1.432	1.028
	2	-1.04		114.0	2.134	1.429	1.009	1.295	-0.135
	3	-0.35	172.7	177.5	1.099	1.214	1.069	1.822	1.285
	4	-0.21	176.7	179.0	1.077	1.201	1.069	2.99	1.775
	5	-0.12	179.1	179.1	1.069	1.207	1.069	3.47	3.205
	6	-0.15	179.7	178.9	1.068	1.207	1.068	3.647	2.609
	7	-0.15	179.5	179.0	1.068	1.207	1.068	3.652	2.619
	8	-0.17	178.3	177.9	1.069	1.212	1.066	2.871	2.651
	9	-0.35	176.8	177.4	1.071	1.213	1.071	2.569	1.728
	10	-0.36	177.5	178.4	1.07	1.213	1.071	2.699	1.544
	11	-0.17	178.3	179.6	1.07	1.207	1.068	3.561	2.860
	12	-0.11	179.6	179.9	1.069	1.207	1.07	3.604	3.473
	13	-0.42	171.9	178.6	1.099	1.215	1.07	1.833	1.293
	14	-0.13	179.9	179.7	1.069	1.207	1.069	3.635	3.459
	15	-0.32	178.1	179.1	1.069	1.211	1.068	2.58	2.147
	16	-0.56		172.2	4.216	1.282	1.083	1.216	-1.977
	17	-0.18		179.1	1.069	1.207	1.067	2.668	1.618
C_2H_2/ZnO (1 1 0)	18	-0.67		177.2	2.108	1.225	1.071	0.999	0.596
	19	-0.68		171.5	2.009	1.235	1.074	2.068	0.563
	20	-0.25		179.6	1.607	1.214	1.069	2.487	1.846
	21	-0.71		174.2	2.034	1.23	1.072	0.999	0.734
	22	-0.72		176.0	2.139	1.225	1.072	0.999	0.482
	23	-0.70		179.5	5.377	1.222	1.072	1.946	0.485
	24	-0.03		177.9	3.6	1.221	1.071	0.991	-2.157
	25	-0.03		174.2	2.543	1.215	1.067	1.296	-0.805
	26	-0.09		179.7	6.266	1.219	1.069	1	-2.243
	27	-0.31		178.1	2.928	1.232	1.066	0.991	0.670
	28	-0.31		178.6	6.253	1.223	1.07	1.009	-2.185
	29	-0.11	179.0	179.8	1.068	1.206	1.068	3.793	3.391
	30	-0.15	177.8	179.0	1.064	1.212	1.071	2.9	2.629
	31	-0.17	178.0	179.7	1.065	1.208	1.071	2.818	2.677
		-0.43	173.1	178.8	1.093	1.215	1.07	3.51	1.326
	33	-0.16	179.5	179.8	1.075	1.207	1.068	2.221	2.267
	34	-0.15	178.5	179.3	1.071	1.208	1.069	3.383	2.822
	35	-0.39	172.4	176.6	1.076	1.215	1.069	2.21	1.878
	36	-0.02	136.7	179.3	3.486	1.222	1.073	0.996	-2.090
	37	-0.19	179.5	178.9	1.083	1.208	1.063	2.089	4.994

	38	-0.50	179.3	176.7	1.109	1.217	1.07	2.331	1.180
	39	-0.11	178.8	179.6	1.071	1.206	1.073	3.324	3.075
	40	-0.16	179.3	179.7	1.077	1.208	1.068	2.05	2.004
	41	-0.21	177.4	179.5	1.077	1.208	1.068	3.064	2.100
	42	-0.17	175.4	179.3	1.071	1.211	1.066	3.27	2.271
	43	-0.43	174.7	178.5	1.096	1.215	1.07	2.408	1.364
	44	-0.16	176.8	178.8	1.069	1.209	1.068	2.477	2.467
	45	-0.27	173.8	179.0	1.083	1.211	1.069	2.562	1.617
	46	-0.33	179.2	178.8	1.069	1.212	1.07	2.562	1.754
	47	-0.18	175.5	178.9	1.081	1.21	1.069	3.151	2.814
	48	-0.25	178.4	179.3	1.069	1.208	1.069	2.845	1.665
C_2H_2/ZnO	49	-0.25	175.6	178.3	1.071	1.211	1.071	2.588	1.780
(1 1 0)	50	-0.42	171.8	177.5	1.09	1.216	1.069	2.435	1.347
	51	-0.36	177.2	179.6	1.082	1.216	1.017	2.426	1.559
	52	-0.19	178.3	179.0	1.071	1.209	1.069	2.951	2.828
	53	-0.11		115.3	4.258	1.358	1.098	0.99	0.285
	54	-0.07		124.0	4.429	1.298	1.087	0.987	-3.448
	55	-0.59		178.5	3.862	1.221	1.086	0.999	0.534
	56	-0.71		177.3	3.628	1.227	1.072	1.006	0.585
	57	-0.09		179.4	3.64	1.22	1.070	0.995	-2.127
	58	-0.69		176.3	2.122	1.224	1.070	1.914	0.450
	59	-1.06		114.4	4.781	1.428	1.100	2.084	-0.060
	60	-0.17		117.0	3.814	1.354	1.101	0.983	-0.356
	61	-0.75		121.3	2.136	1.36	1.096	2.045	-0.293
	62	-0.75		175.5	3.409	1.224	1.082	1.014	-2.074
	63	-0.50	178.0	178.2	1.106	1.216	1.07	2.39	1.164
	64	-1.15	123.7	113.1	1.097	1.332	1.094	1.951	1.115
	65	-0.84	126.1	118.2	1.096	1.331	1.092	1.412	1.249
	66	-0.31	175.7	178.9	1.072	1.211	1.070	2.481	1.713
	67	-0.46	174.4	178.9	1.099	1.216	1.071	3.133	1.162
	68	-0.14	179.1	179.0	1.071	1.207	1.068	3.342	3.017
	69	-0.30	175.2	176.9	1.076	1.208	1.068	2.529	1.665
	70	-0.97	125.8	117.4	1.097	1.332	1.091	1.407	1.014
	71	-0.20	178.1	179.0	1.073	1.21	1.065	3.009	2.784
	72	-0.31	177.7	177.4	1.609	1.211	1.07	2.535	1.802
	73	-0.09	178.4	177.9	1.069	1.209	1.071	3.126	2.734
	74	-1.12	123.5	112.3	1.097	1.333	1.096	2.950	1.137
	75	-0.28	174.2	179.4	1.085	1.214	1.070	2.517	1.449

* Parameters: BE, binding energy; ∠HCC, the angle of HCC in acetylene; ∠HCC, the angle of CCH in acetylene; d(ads-sub), shortest adsorbate-substrate distance; d⊥(ads-sub), shortest perpendicular height of bent or discomposed acetylene above

the top ZnO surface layer.

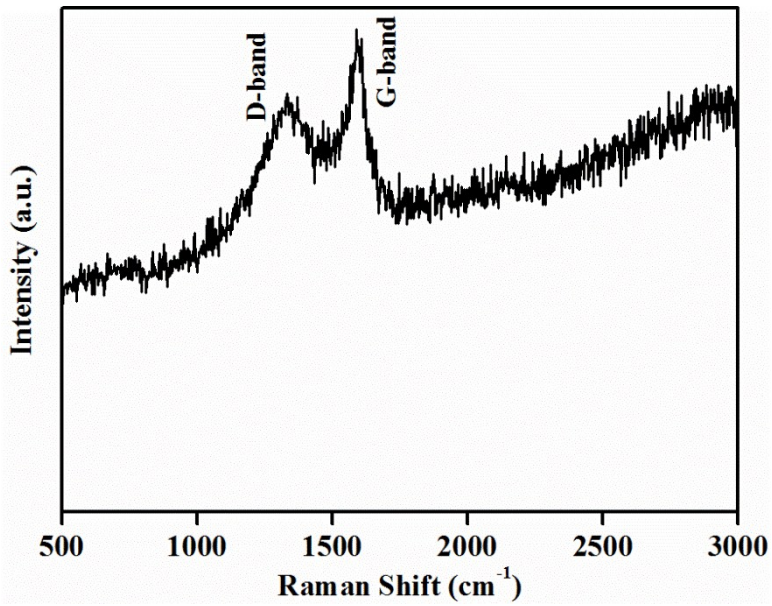

Figure S6. The Raman spectra of GCs@T-ZnO prepared at 700 °C.

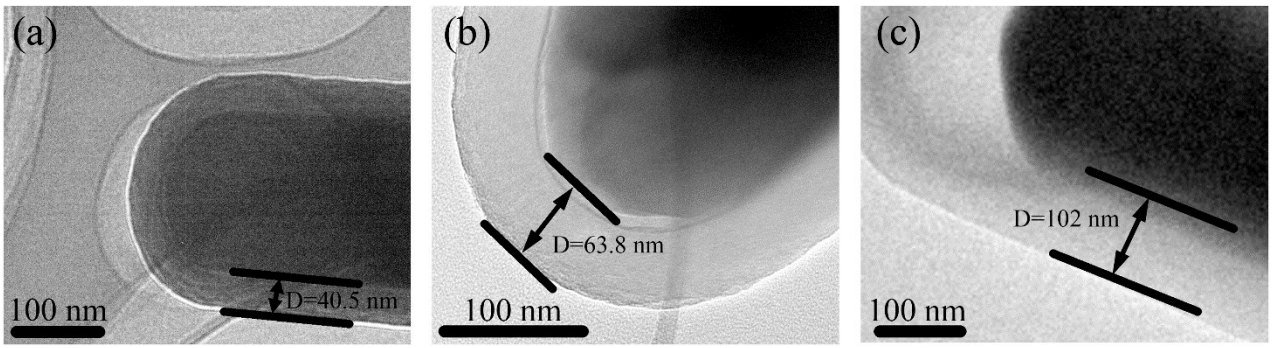

Figure S7. The TEM images of GC@T-ZnO prepared at 700 °C under different acetylene flow rates (a) 20 mL/min, (b) 40 mL/min and (c) 60 mL/min.