

Supplementary part:

Table 1S. The averaged values of commonly used parameters for the characterization of the DNA geometry for each base step of ds-DNA (shift to twist) and each base pair (buckle, propeller). The values for the free ds-DNA are depicted first, followed by those for the anchored DNA on the graphene slab with various charge.

Free ds-DNA	1	2	3	4	5	6	7	8	9	10
shift	-0.10	-0.19	0.05	0.33	-0.07	-0.24	-0.07	0.20	0.13	-
slide	-0.96	-0.42	-0.84	-0.94	-0.57	-0.98	-0.82	-0.45	-1.00	-
rise	3.53	3.26	3.35	3.36	3.27	3.35	3.34	3.28	3.53	-
tilt	-1.16	0.40	-2.36	2.68	-0.08	-2.41	2.31	-0.11	1.26	-
roll	6.41	9.22	0.50	3.31	10.91	3.26	0.43	9.28	6.61	-
twist	32.22	29.39	32.46	31.72	29.57	31.36	32.57	29.59	31.95	-
buckle	5.00	-2.13	0.36	1.44	-0.78	-0.19	-1.72	0.04	1.42	-5.86
propeller	-15.03	-9.18	-9.69	-10.70	-13.10	-12.81	-10.63	-9.24	-9.39	-15.01
gra-0.1	1	2	3	4	5	6	7	8	9	10
shift	0.69	-0.32	0.63	0.57	0.13	-0.53	-0.36	0.11	0.15	-
slide	-0.38	-0.04	-0.70	-1.01	-1.33	-1.61	-0.97	-0.39	-0.76	-
rise	3.49	3.28	3.25	3.27	3.48	3.51	3.34	3.26	3.51	-
tilt	-1.90	-2.13	-2.45	2.53	0.58	-1.41	1.30	-0.09	1.18	-
roll	6.06	12.90	3.93	6.58	12.28	1.57	-0.89	7.48	5.33	-
twist	34.04	29.89	30.86	28.10	29.32	28.81	32.00	31.78	32.00	-
buckle	-4.04	-7.86	-1.83	4.43	8.19	-1.92	-7.64	-4.01	-0.07	-4.93
propeller	-17.15	-12.05	-9.87	-6.38	-13.19	-13.92	-9.10	-7.57	-9.13	-13.25
gra-0.05	1	2	3	4	5	6	7	8	9	10
shift	0.02	-0.23	0.02	0.28	0.03	-0.38	0.03	0.21	0.10	-
slide	-1.00	-0.38	-0.85	-0.96	-0.59	-0.89	-0.78	-0.40	-0.95	-
rise	3.54	3.26	3.37	3.38	3.28	3.39	3.36	3.27	3.55	-
tilt	-1.23	0.01	-2.14	2.25	-0.05	-2.45	2.24	-0.18	1.19	-
roll	5.01	8.62	0.25	2.93	10.20	3.01	0.12	9.37	6.31	-
twist	31.45	29.84	32.50	31.54	29.52	32.22	32.71	29.22	31.70	-
buckle	4.35	-2.27	1.16	2.13	0.05	0.78	-1.94	-0.68	1.74	-5.25

propeller	-12.43	-8.18	-9.05	-11.00	-12.71	-13.32	-11.17	-9.40	-8.76	-14.73
gra-0.02	1	2	3	4	5	6	7	8	9	10
shift	-3.38	-0.11	-0.06	0.15	0.03	-0.37	-0.03	0.21	0.09	-
slide	-1.98	-0.53	-0.91	-1.03	-0.55	-0.96	-0.77	-0.42	-0.99	-
rise	1.60	3.25	3.38	3.36	3.31	3.41	3.35	3.25	3.55	-
tilt	37.98	0.56	-2.08	1.73	-0.15	-2.46	2.06	-0.34	1.12	-
roll	-32.76	7.51	-0.21	2.25	8.50	2.76	0.13	9.43	6.65	-
twist	-18.27	29.91	32.51	30.43	31.16	32.10	32.70	29.14	32.02	-
buckle	-4.25	-3.58	0.76	1.71	1.65	1.63	-2.29	-0.73	2.20	-5.18
propeller	-19.70	-5.91	-8.97	-9.72	-11.80	-13.62	-11.02	-9.16	-9.21	-15.22
gra-0.01	1	2	3	4	5	6	7	8	9	10
shift	-0.02	-0.26	-0.02	0.30	-0.01	-0.42	-0.03	0.30	1.98	-
slide	-1.07	-0.43	-0.85	-0.88	-0.52	-0.88	-0.77	0.06	-0.88	-
rise	3.51	3.27	3.38	3.37	3.28	3.44	3.41	3.19	3.46	-
tilt	-0.95	0.22	-2.19	2.45	0.01	-2.58	1.90	2.15	-1.71	-
roll	5.19	7.99	-0.51	2.72	10.24	3.19	-0.80	4.56	4.24	-
twist	30.82	29.79	32.67	31.79	29.15	32.73	33.40	29.49	81.93	-
buckle	2.66	-2.65	0.82	1.26	-0.09	0.85	-4.33	-4.80	5.18	22.40
propeller	-11.29	-7.42	-8.78	-10.84	-12.04	-14.21	-12.47	-7.61	1.72	-16.24
gra0	1	2	3	4	5	6	7	8	9	10
shift	-0.34	-0.23	-0.16	0.19	-0.02	-0.31	-0.07	0.20	0.14	-
slide	-1.50	-0.74	-0.99	-1.00	-0.59	-0.97	-0.85	-0.50	-1.08	-
rise	3.44	3.57	3.42	3.39	3.28	3.38	3.33	3.29	3.55	-
tilt	-0.96	-0.90	-2.57	1.60	-0.04	-2.51	2.23	-0.31	1.45	-
roll	5.98	8.90	0.03	2.71	9.67	2.90	0.95	9.80	6.69	-
twist	32.13	31.69	32.42	30.77	30.01	31.66	32.11	29.74	31.82	-
buckle	13.11	9.85	1.69	0.87	-0.52	0.58	-1.64	0.27	1.14	-6.58
propeller	-9.00	-11.23	-9.81	-10.12	-11.66	-12.84	-10.40	-9.77	-9.75	-14.98
gra+0.01	1	2	3	4	5	6	7	8	9	10
shift	-0.29	-0.29	0.29	0.28	-0.01	-0.21	-0.24	0.23	0.11	-
slide	-0.48	-0.88	-1.08	-1.28	-0.93	-1.26	-0.99	-0.48	-0.98	-
rise	3.33	3.62	3.32	3.32	3.30	3.35	3.34	3.29	3.55	-
tilt	-2.16	0.51	-2.90	2.87	0.52	-1.72	2.14	-0.21	1.39	-

roll	13.69	16.73	3.41	3.54	11.84	2.50	1.11	9.40	6.36	-
twist	35.33	29.57	29.98	29.26	29.17	29.52	31.44	29.83	31.86	-
buckle	11.92	10.24	-4.75	-1.77	-1.46	-2.86	-2.68	-0.25	1.34	-6.22
propeller	-5.14	-17.50	-11.30	-7.16	-11.46	-11.81	-8.65	-8.64	-9.29	-14.62
gra+0.02	1	2	3	4	5	6	7	8	9	10
shift	-0.28	-0.25	0.93	0.13	0.20	-0.29	-0.20	0.04	0.02	-
slide	-1.65	-0.90	-1.30	-1.50	-0.98	-1.40	-0.80	-0.43	-0.95	-
rise	3.48	3.60	3.31	3.17	3.31	3.45	3.35	3.19	3.57	-
tilt	-1.97	1.11	-3.11	3.62	1.24	-1.12	1.81	-0.10	1.36	-
roll	14.11	23.72	6.24	6.40	16.92	3.31	-1.68	7.01	6.13	-
twist	29.12	25.98	29.05	25.00	26.76	30.77	32.68	27.16	32.73	-
buckle	15.84	6.46	-6.95	-4.68	0.76	-2.94	-7.82	-4.32	2.27	-6.15
propeller	-13.51	-15.68	-13.48	-5.11	-10.96	-15.55	-10.42	-5.20	-8.67	-15.48
gra+0.05	1	2	3	4	5	6	7	8	9	10
shift	-0.18	-0.61	0.89	0.28	-1.61	0.55	-0.12	0.26	0.18	-
slide	0.16	0.63	-0.72	-0.52	0.35	-0.06	0.11	-0.20	-0.02	-
rise	3.23	3.20	3.42	3.55	3.28	3.40	3.57	3.33	3.43	-
tilt	-3.48	-0.55	-2.17	4.09	-2.36	-0.96	0.75	-0.57	2.07	-
roll	5.43	10.20	0.73	-3.68	-6.39	-2.44	-11.64	8.28	5.76	-
twist	27.04	28.84	37.58	33.09	34.31	33.41	37.59	30.01	30.21	-
buckle	-16.57	-4.37	6.28	2.24	-2.33	1.91	2.11	-4.19	-4.44	-3.52
propeller	-13.11	-10.35	-16.11	-18.08	-5.97	-19.81	-16.82	-15.21	-10.73	-12.31
gra+0.1	1	2	3	4	5	6	7	8	9	10
shift	0.28	-0.21	0.03	0.38	0.08	-0.75	-0.50	0.46	0.70	-
slide	-0.72	-0.33	-0.89	-0.72	-0.64	-1.05	-1.07	-0.20	-0.51	-
rise	3.51	3.32	3.42	3.37	3.14	3.48	3.46	3.40	3.70	-
tilt	-0.15	0.32	-2.26	2.44	-0.19	-3.41	1.96	0.64	4.99	-
roll	4.62	8.01	-0.27	0.24	11.72	3.03	0.51	8.81	7.05	-
twist	32.28	30.04	32.72	32.44	21.65	32.04	32.53	30.34	27.73	-
buckle	2.68	-3.01	-1.73	-2.51	-1.32	7.26	1.00	-2.36	-3.24	-11.97
propeller	-14.03	-9.53	-10.78	-11.37	-7.43	-10.95	-13.70	-13.49	-8.57	-16.46

Table 2S. The averaged values of commonly used parameters for the characterization of the DNA geometry for each base step of ss-DNA. The values for the free ss-DNA are depicted first, followed by those for the anchored DNA on the graphene slab with various charge.

Free ss-DNA	1	2	3	4	5	6	7	8	9
shift	2.10	3.75	2.07	2.89	2.79	2.80	2.24	1.87	0.21
slide	1.45	1.24	-0.20	-0.16	1.10	0.75	-0.18	0.55	0.76
rise	2.56	3.27	3.65	3.60	3.16	3.32	3.19	1.82	1.87
tilt	-49.46	6.43	-2.99	0.92	11.18	4.30	6.03	4.06	-3.43
roll	95.20	10.63	12.05	9.63	4.94	8.85	7.14	4.61	5.69
twist	-4.40	52.99	39.43	47.37	47.68	48.00	41.39	32.20	7.25
gra-0.1	1	2	3	4	5	6	7	8	9
shift	1.06	2.32	-4.78	3.16	4.82	-1.59	-9.07	-1.21	0.95
slide	0.24	1.56	-0.48	-0.36	3.91	1.14	-2.19	0.75	2.76
rise	3.37	3.81	0.52	3.79	4.25	3.08	2.04	-1.49	1.28
tilt	6.15	2.34	37.60	-2.07	-1.35	9.03	10.07	56.66	0.17
roll	12.30	24.35	-59.30	8.62	44.91	7.21	-29.13	-14.38	14.24
twist	31.69	37.26	-7.01	46.69	81.41	-14.88	-33.52	-7.19	26.71
gra-0.05	1	2	3	4	5	6	7	8	9
shift	-4.23	3.53	1.98	3.07	3.48	3.10	2.19	2.44	-2.79
slide	-1.57	1.10	-0.21	-0.12	1.33	0.76	0.09	1.29	0.69
rise	4.36	3.62	3.56	3.37	3.40	3.31	2.93	4.09	1.53
tilt	-42.67	2.43	0.37	4.55	8.56	4.46	9.37	4.36	35.45
roll	-9.01	11.86	9.45	8.57	5.96	10.68	3.29	0.48	-41.50
twist	-17.76	54.54	39.23	47.66	58.56	48.66	40.62	44.10	3.99
gra-0.02	1	2	3	4	5	6	7	8	9
shift	0.63	-1.60	-5.66	2.73	3.46	1.96	1.04	1.82	-5.98
slide	0.12	0.81	-1.37	-0.06	1.35	0.86	2.03	0.67	-0.66
rise	5.86	0.50	3.32	3.84	3.39	2.23	2.41	1.37	-0.14
tilt	-26.25	45.59	-1.54	-0.60	8.52	7.29	8.66	0.52	75.68
roll	31.32	-34.91	-22.95	8.44	6.50	20.56	-3.84	23.41	-62.46
twist	27.91	21.36	-18.05	45.71	56.70	42.30	10.97	27.96	-43.17
gra-0.01	1	2	3	4	5	6	7	8	9
shift	2.74	3.19	-1.00	2.86	4.10	2.27	2.78	2.31	1.20
slide	0.55	1.68	-0.99	-0.24	2.18	0.79	-0.08	1.19	0.80
rise	5.27	3.72	4.53	3.74	3.96	3.32	3.21	3.51	3.38
tilt	-12.55	0.50	-19.13	0.07	0.49	3.40	5.31	6.32	6.28
roll	14.50	19.67	11.22	6.93	25.34	10.43	8.70	9.64	6.65
twist	57.65	50.00	9.12	46.45	66.13	41.40	44.34	44.98	20.89
gra0	1	2	3	4	5	6	7	8	9
shift	2.86	2.51	-3.14	2.00	1.46	1.65	2.30	3.53	1.35
slide	0.93	1.76	-0.88	0.27	0.25	0.85	-0.32	1.59	0.72
rise	7.04	3.81	1.56	5.89	0.72	1.15	3.27	3.40	3.20
tilt	-27.80	0.07	21.06	-17.93	1.81	-19.60	4.93	9.69	8.86
roll	10.95	21.01	-21.96	0.53	1.13	54.00	6.10	8.78	6.30
twist	60.97	44.76	1.09	30.81	22.44	-8.39	42.23	58.50	23.83
gra+0.01	1	2	3	4	5	6	7	8	9
shift	-9.11	-6.52	-10.26	-8.35	-5.22	1.12	-4.61	3.09	-0.01
slide	-3.18	-0.97	-3.41	-2.82	-1.83	0.34	-3.63	0.75	1.72
rise	0.46	0.42	0.30	1.17	1.09	3.48	1.08	3.17	-0.38
tilt	-2.24	-0.76	3.96	2.15	-0.79	7.83	34.78	7.44	42.03
roll	0.70	-0.13	-4.38	-3.95	1.45	3.57	44.58	4.47	-13.89
twist	-22.88	-2.79	-35.97	-20.98	2.92	36.22	-33.10	54.12	-19.86
gra+0.02	1	2	3	4	5	6	7	8	9
shift	-2.02	-2.24	0.56	-0.46	-0.91	-0.25	2.36	-1.97	-7.51
slide	-1.33	1.43	-0.58	-1.62	0.28	1.02	-0.36	1.90	-3.54
rise	6.22	-4.60	3.51	7.55	-0.21	2.74	3.28	5.62	-4.20
tilt	-22.47	25.09	14.93	-27.85	48.74	8.70	4.50	-12.88	27.89
roll	-8.17	18.22	-16.52	-15.33	-34.88	-13.88	3.51	12.62	42.31
twist	18.57	29.97	31.09	25.43	28.85	30.33	43.54	-17.66	-50.48
gra+0.05	1	2	3	4	5	6	7	8	9
shift	1.82	4.25	1.96	-8.39	3.03	1.19	-3.19	2.75	0.64
slide	0.26	0.53	1.70	-1.75	0.35	0.38	-1.00	0.97	0.84
rise	3.36	3.46	5.41	6.43	3.79	3.35	3.20	3.11	3.02
tilt	4.45	3.22	-27.49	-60.84	-2.05	6.53	11.41	10.67	14.78
roll	6.70	9.73	48.03	56.39	7.41	14.03	10.81	15.39	6.93
twist	36.47	56.98	35.58	-49.74	52.17	37.57	-9.83	43.34	25.52
gra+0.1	1	2	3	4	5	6	7	8	9
shift	2.66	2.72	3.11	0.62	2.32	-1.81	1.29	1.66	0.44
slide	-0.04	1.76	0.56	3.10	0.91	-0.91	-0.47	1.33	0.78

rise	3.75	3.51	5.94	0.02	1.38	3.83	3.28	3.61	7.95
tilt	0.77	5.99	-37.58	13.51	-17.96	2.79	5.56	6.68	-28.70
roll	8.49	8.12	33.52	-2.59	56.97	2.65	3.89	11.96	-31.12
twist	46.79	50.56	48.80	20.90	11.88	9.69	36.03	32.02	-26.82