Support information

Table S1. The number of molecules in each system

Type of peptides	Number of peptides	Number of sodium ions	Number of chloride ions	Number of water
ARG3	20	10	70	17250
	40	10	130	16879
	60	10	190	16508
	80	10	250	16137
ARG7	20	10	150	16644
	40	10	290	15666
	60	10	430	14688
	80	10	570	13711
ARG11	20	10	230	16123
	40	10	450	14624
	60	10	670	13126
	80	10	890	11627
LYS3	20	10	70	17284
	40	10	130	16947
	60	10	190	16611
	80	10	250	16274
LYS7	20	10	150	16743
	40	10	290	15865
	60	10	430	14987
	80	10	570	14109
LYS11	20	10	230	16278
	40	10	450	14934
	60	10	670	13590
	80	10	890	12247
ASN3	20	10	10	17412
	40	10	10	17202
	60	10	10	16993
	80	10	10	16783
ASN7	20	10	10	17138
	40	10	10	16655
	60	10	10	16172
	80	10	10	15689
ASN11	20	10	10	16868
	40	10	10	16114
	60	10	10	15361
	80	10	10	14607
GLN3	20	10	10	17379
	40	10	10	17136
	60	10	10	16894
	80	10	10	16651
GLN7	20	10	10	16993
	40	10	10	16364
	60	10	10	15735

	80	10	10	15106
GLN11	20	10	10	16650
	40	10	10	15680
	60	10	10	14709
	80	10	10	13738
TRP3	20	10	10	17261
	40	10	10	16901
	60	10	10	16541
	80	10	10	16181
TRP7	20	10	10	16609
	40	10	10	15598
	60	10	10	14586
	80	10	10	13574
TRP11	20	10	10	16094
	40	10	10	14567
	60	10	10	13040
	80	10	10	11513
HIS3	20	10	10	17364
	40	10	10	17107
	60	10	10	16849
	80	10	10	16592
HIS7	20	10	10	16922
	40	10	10	16223
	60	10	10	15523
	80	10	10	14824
HIS11	20	10	10	16541
	40	10	10	15461
	60	10	10	14381
	80	10	10	13300
ALA3	20	10	10	17472
	40	10	10	17323
	60	10	10	17174
	80	10	10	17026
ALA7	20	10	10	17277
	40	10	10	16932
	60	10	10	16587
	80	10	10	16243
ALA11	20	10	10	17102
	40	10	10	16583
	60	10	10	16064
	80	10	10	15545
ILE3	20	10	10	17368
	40	10	10	17114
	60	10	10	16861
	80	10	10	16607
ILE7	20	10	10	16927
	40	10	10	16232
	60	10	10	15538
	80	10	10	14843

ILE11	20	10	10	16548
	40	10	10	15475
	60	10	10	14402
	80	10	10	13329
ASP3	20	70	10	17415
	40	130	10	17208
	60	190	10	17002
	80	250	10	16795
ASP7	20	150	10	17040
	40	290	10	16459
	60	430	10	15878
	80	570	10	15297
ASP11	20	230	10	16728
	40	450	10	15834
	60	670	10	14940
	80	890	10	14047
GLU3	20	70	10	17378
	40	130	10	17136
	60	190	10	16893
	80	250	10	16650
GLU7	20	150	10	16980
	40	290	10	16339
	60	430	10	15698
	80	570	10	15057
GLU11	20	230	10	16613
	40	450	10	15604
	60	670	10	14595
	80	890	10	13586
PVP3	20	10	10	17393
	40	10	10	17166
	60	10	10	16938
	80	10	10	16710
PVP6	20	10	10	17096
	40	10	10	16571
	60	10	10	16047
	80	10	10	15522
PV10	20	10	10	16740
	40	10	10	15858
	60	10	10	14977
	80	10	10	14095

Table. S2. Intermolecular interaction energies of peptide-graphene and peptide-water in the system with polymerization degree 11 and peptide number 60 (Unit: kJ·mol^{-1})

	E_{vdW}	E_{elec}	E_{total}(peptide-graphene)	E_{vdW}	E_{elec}	E_{total}(peptide-water)
ARG	-1243	0	-1243	-440	-210687	-211127
LYS	-1085	0	-1085	-4582	-202978	-207560
ASN	-1635	0	-1635	-7441	-111567	-119008
GLN	-1520	0	-1520	-9440	-114649	-124089
TRP	-1668	0	-1668	-19171	-110300	-129471
HIS	-1392	0	-1392	-10495	-113713	-124208
ALA	-1137	0	-1137	-7557	-70145	-77702
ILE	-1297	0	-1297	-12023	-77017	-89040
ASP	-556	0	-556	2983	-319809	-316826
GLU	-568	0	-568	2629	-314694	-312065
PVP	-1098	0	-1098	-15110	-47370	-62480

Fig. S1. Displacement of the centroids of adjacent graphenes in the yz plane during NVT

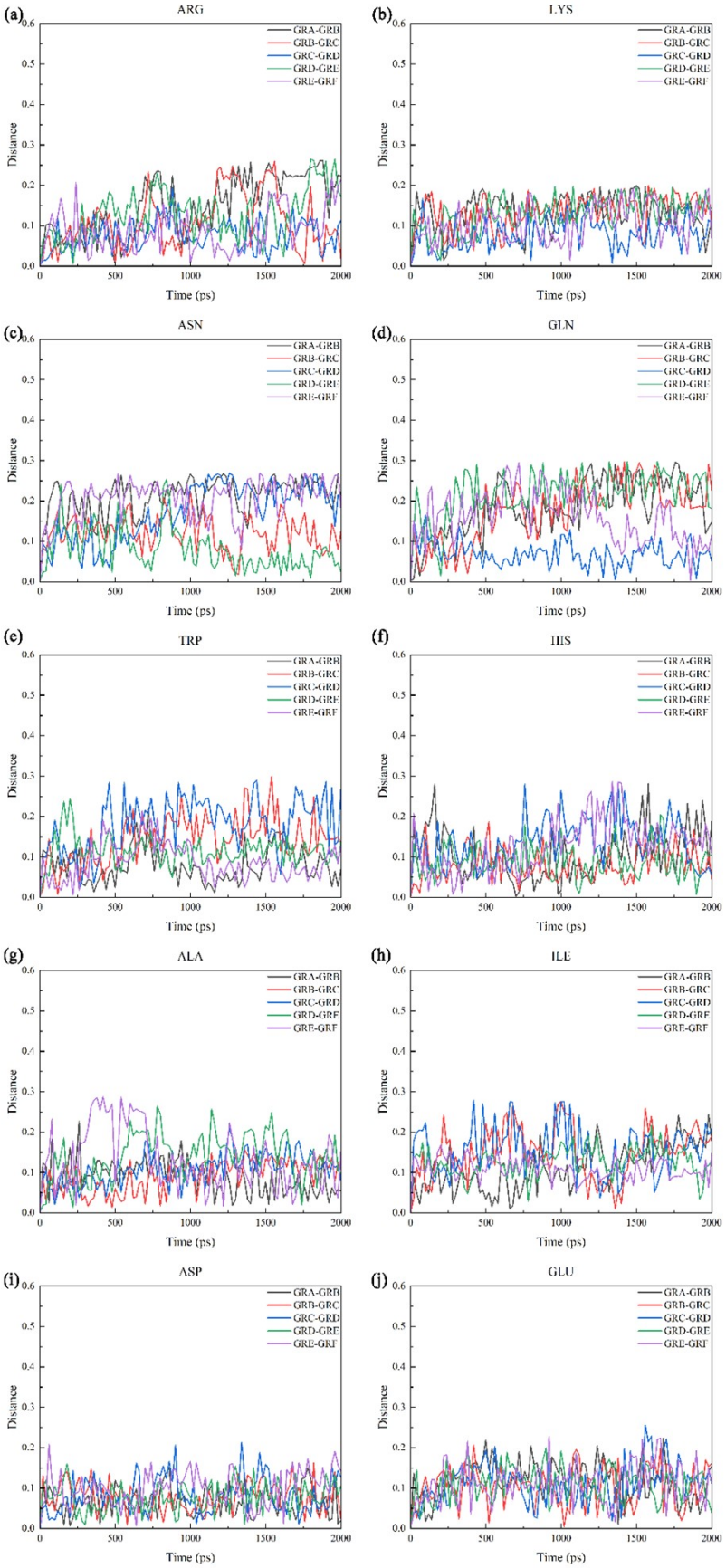

Fig. S2. Monomer structures of different peptides (a)ARG (b)LYS (c)ASN (d)GLN (e)HIS (f)TRP (g)ALA (h) ILE (i)ASP (j) GLU

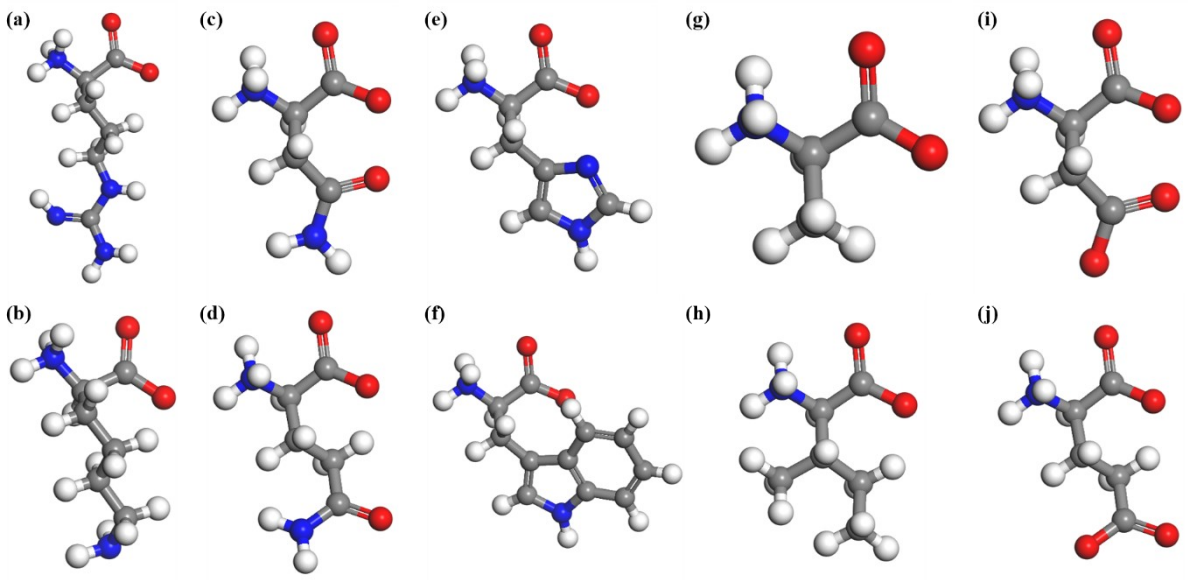

Fig. S3. Schematic diagram of the radial distribution function (RDF) of different atom pairs in the peptide-graphene-water system.