Table S1. Examples of pH stimuli-responsive drug delivery systems for DOX.

carrier	Functional group	references
Graphene	-	34
Graphene oxide	-	34
carbon nanotube	chitosan	60
carbon nanotube	·OOC(e)-CNT, OH (e) – CNT, H2N(e) - CNT	61
Graphene	Folic acid	62
carbon nanotube	N-isopropyl acrylamide Carbon	63
black phosphorus	polyethylenimine	45
Graphene oxide	Polyethylene glycol	64

Table S2. Details of the designed simulation boxes.

System	*carrier*	*pH*	*DOX*	*No. Water molecules*	*Box Size (nm3)*
pGOX/DOX	graphene oxide	5.0	4	12084	8.00×8.00×6.00
GOX/DOX	graphene oxide	7.4	4	12166	8.00×8.00×6.00
pGOX/PMLA-ami-DOX	graphene oxide	5.0	4	12037	8.00×8.00×6.00
GOX/PMLA-ami-DO X	graphene oxide	7.4	4	12057	8.00×8.00×6.00
pGOX/PMLA-hz-DOX	graphene oxide	5.0	4	12034	8.00×8.00×6.00
GOX/PMLA-hz-DOX	graphene oxide	7.4	4	12124	8.00×8.00×6.00

Table S3. A summary of MD simulation's states.

Stage	*Time(ns)*	*Time step (fs)*
NVT	0.2	0.0002
NpT	0.2	0.0002
MD	105	0.0015

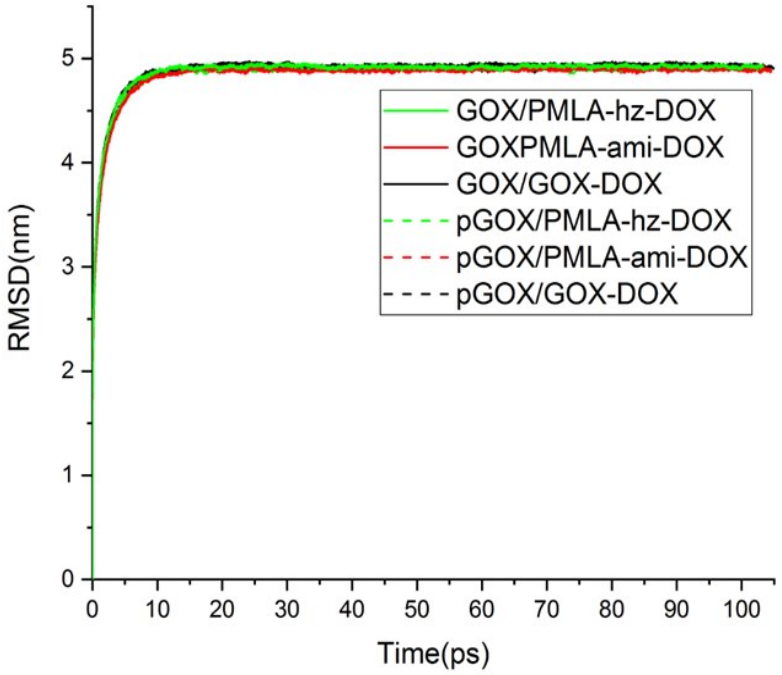
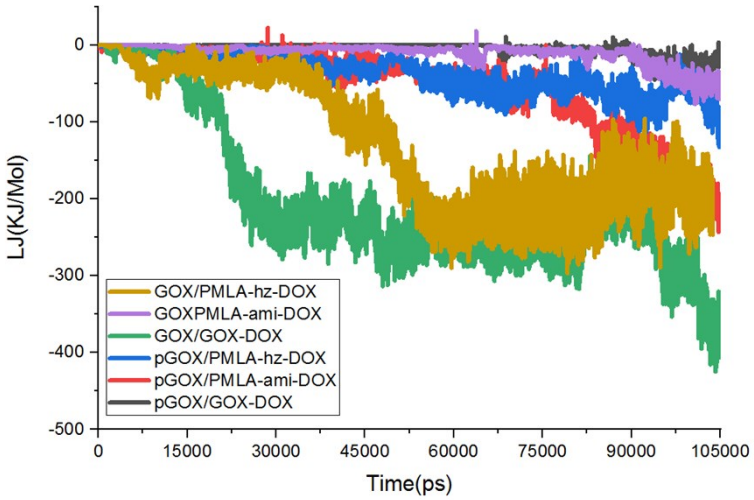


Figure S1. RMSD curves for the simulation systems at different pHs.



FigureS2. The LJ interaction energies of guest molecules and GO interactions in pH level.

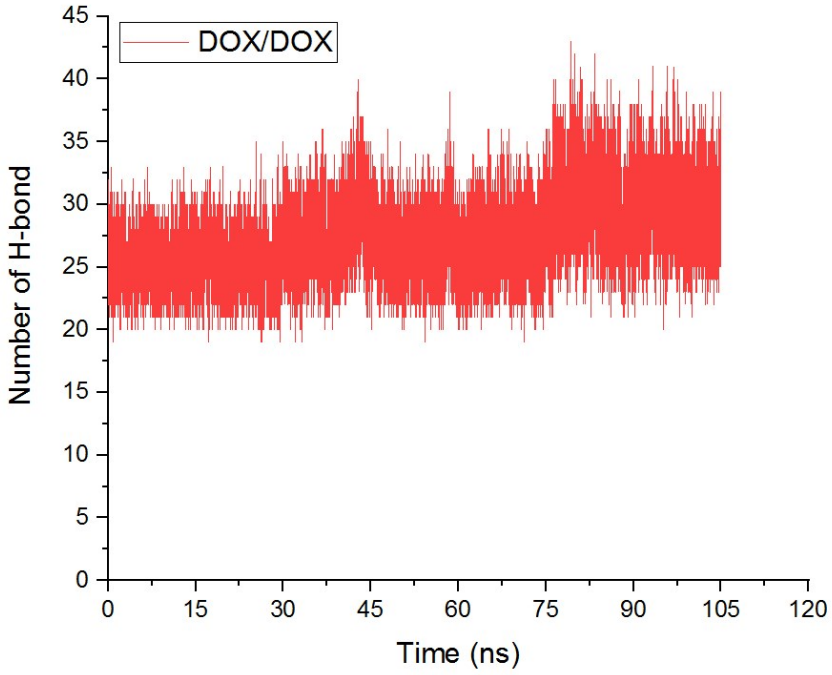


Figure S3. The number of hydrogen bond between DOX-DOX molecules in the pGOX / DOX system.

Figure S4. The average number of hydrogen bonds in simulation time, between guest molecules and GOX surface, guest molecules and water, GOX and water.

system	pair	Average value
GOX/DOX	GOX-DOX	7.466
	DOX-Sol	138.608
	GOX-Sol	822.704
pGOX/DOX	GOX-DOX	0.067
	DOX-Sol	130.851
	GOX-Sol	805.180
pGOX/PMLA-hz-DOX	GOX-DOX	3.556
	DOX-Sol	277.184
	GOX-Sol	806.888
GOX/PMLA-hz-DOX	GOX-DOX	7.809
	DOX-Sol	222.998
	GOX-Sol	829.263