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# Designing a pH-responsive drug delivery system based on smart polymer coating of graphene nanosheet: A theoretical study

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**Figure S1.** The initial sturuce of A) graphene, B) DOX, and C) PEI molecules.

**Figure S2**. Close snapshots from the orientation of DOX molecule of graphene in A) G-DOX and B) G-pDOX systems. The DOX molecule is drawn in form of ball and stick type, while the graphene is drawn in tube form.

**Figure S3.** A) The RDF plot between drug molecule and graphene, B) atomic RDF between N atom of DOX and graphene and C) The density profile of drug molecule around of graphene surface.

**Figure S4.** The number of hydrogen bond between A) PEI and DOX and B) PEI and water in G-DOX@PEI and G-pDOX@pPEI systems.

**Table S1.** Details of the MD simulation systems.

**Table S2**. The non-bonded parameters set for graphene employed for all reported simulations.

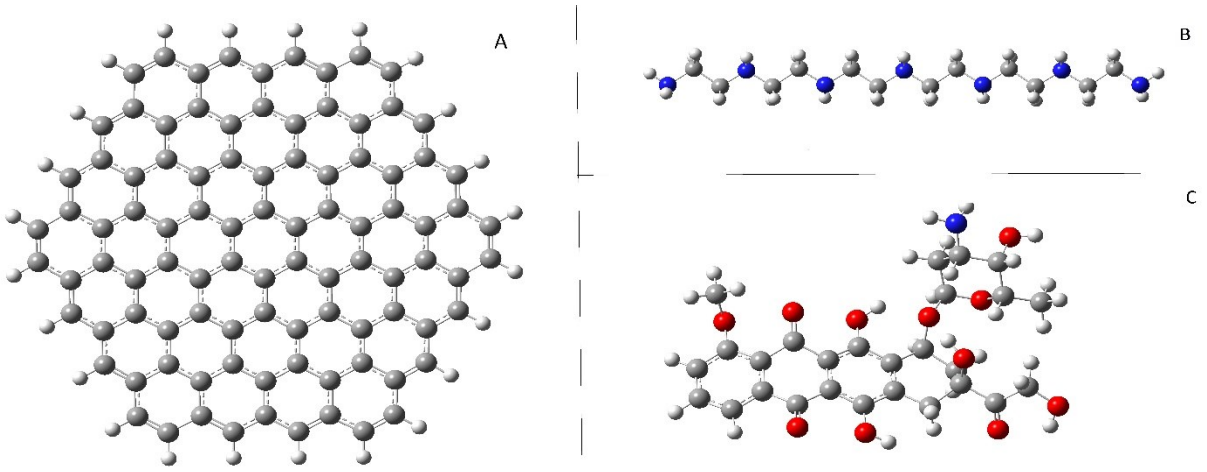


*Figure S1 .The structure of A) graphene, B) DOX, and C) PEI molecules.*

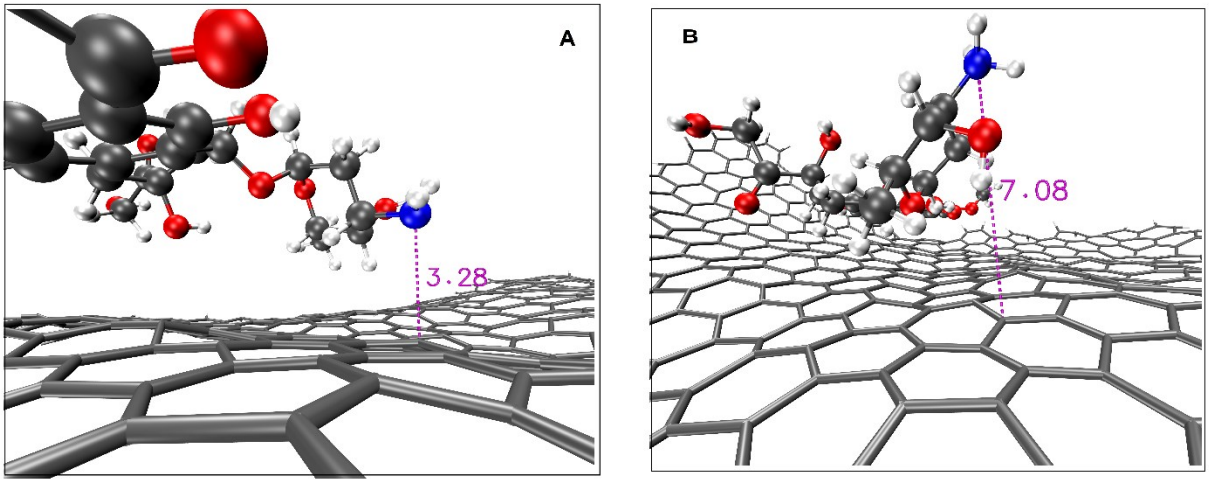


Figure S2. Close snapshots from the orientation of DOX molecule of graphene in A) G-DOX and B) G-pDOX systems. The DOX molecule is drawn in form of ball and stick type, while the graphene is drawn in tube form.

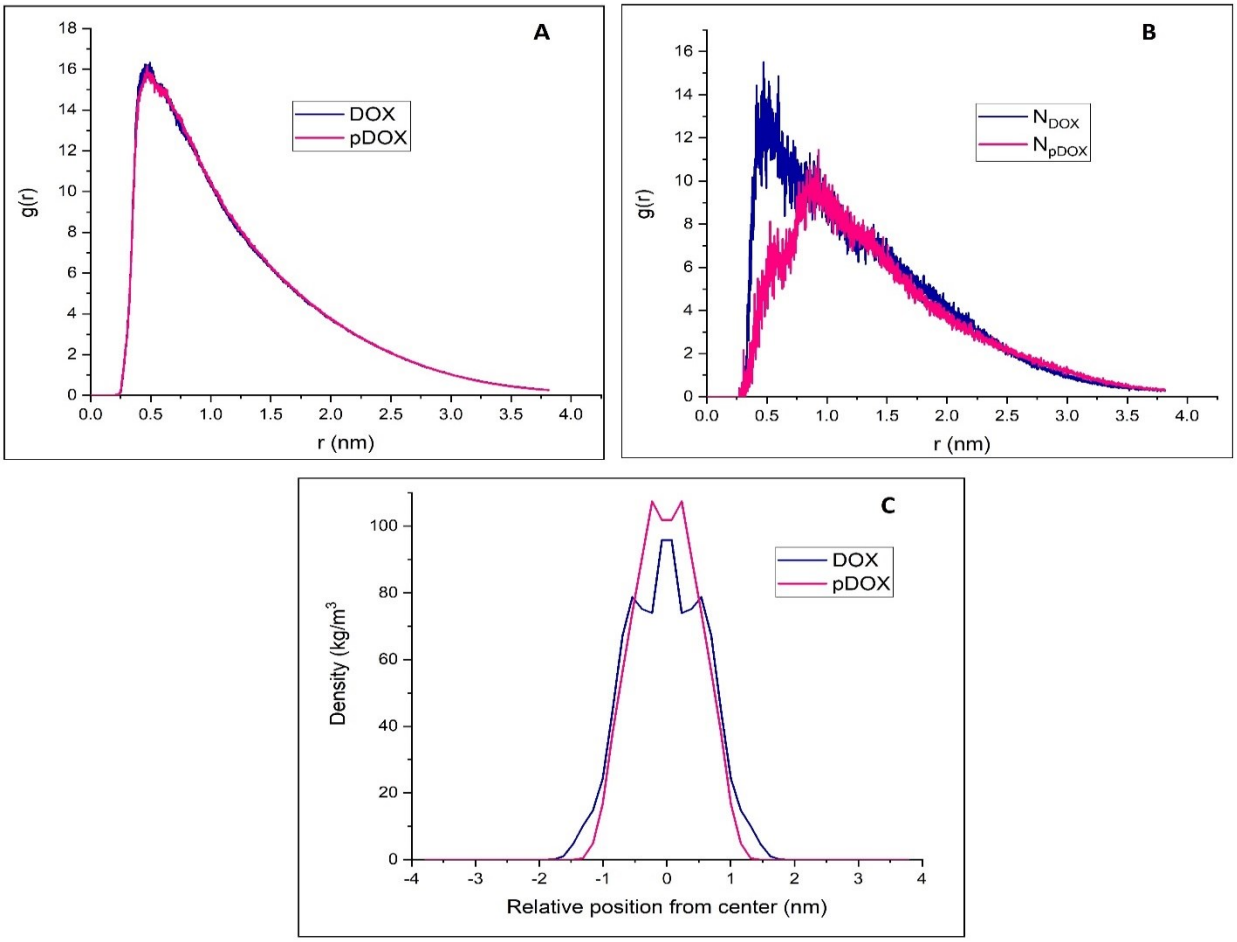


**Figure S3.** A) The RDF plot between drug molecule and graphene, B) atomic RDF between N atom of DOX and graphene and C) The density profile of drug molecule around of graphene surface in G-DOX and G-pDOX systems.

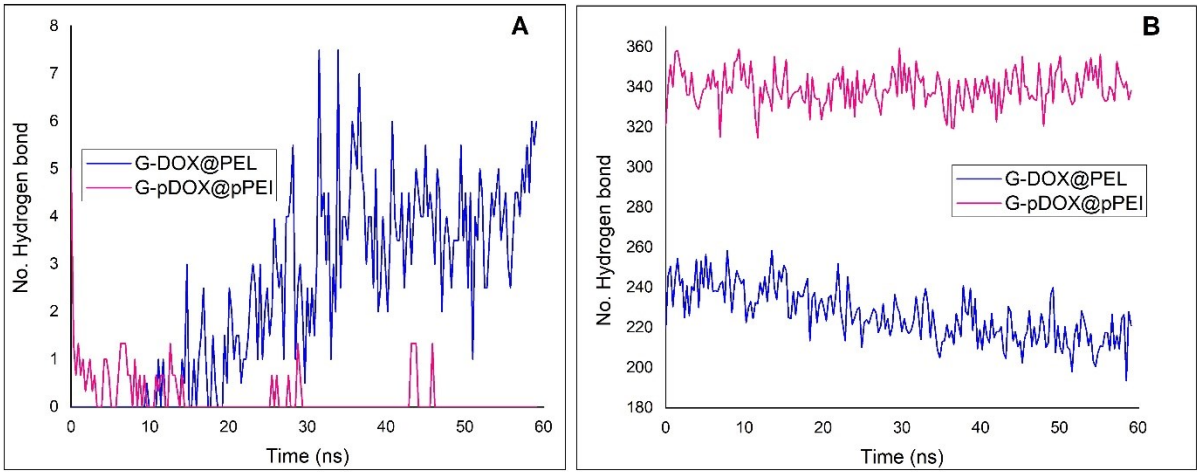


**Figure S4.** A) The number of hydrogen bonds between A) PEI and DOX and B) PEI and water in G-DOX@PEI and G-pDOX@pPEI systems.

**Table S1.** Details of the MD simulation systems.

| MD simulation box | No. of carrier (No. of atoms) | No. DOX (No. of atoms) | No. PEI chain (No. of atoms) | No. of water molecules | No. of total atoms | Box Size ($nm^3$) |
|---|---|---|---|---|---|---|
| G-DOX | 1 (750 atoms) | 10 (670 atoms) | - | 16344 | 50452 | 8×8×8 |
| G-pDOX | 1 (750 atoms) | 10 (680 atoms) | - | 16351 | 50483 | 8×8×8 |
| G-DOX@PEI | 1 (750 atoms) | 10 (670 atoms) | 10 (520 atoms) | 16170 | 50450 | 8×8×8 |
| G-pDOX@pPEI | 1 (750 atoms) | 10 (680 atoms) | 10 (590 atoms) | 16139 | 50437 | 8×8×8 |

Table S2. The non-

| | Atom | Sigma (A˚) | Epsilon (kj/mol) |
|---|---|---|---|
| Graphene | C | 0.35500 | 0.29288 |
| | H | 0.24200 | 0.12552 |

bonded parameters set for graphene employed for all reported simulations.