

Support Information

Theoretical Evaluation of Potential Cytotoxicity of Graphene Quantum Dot to Adsorbed DNA

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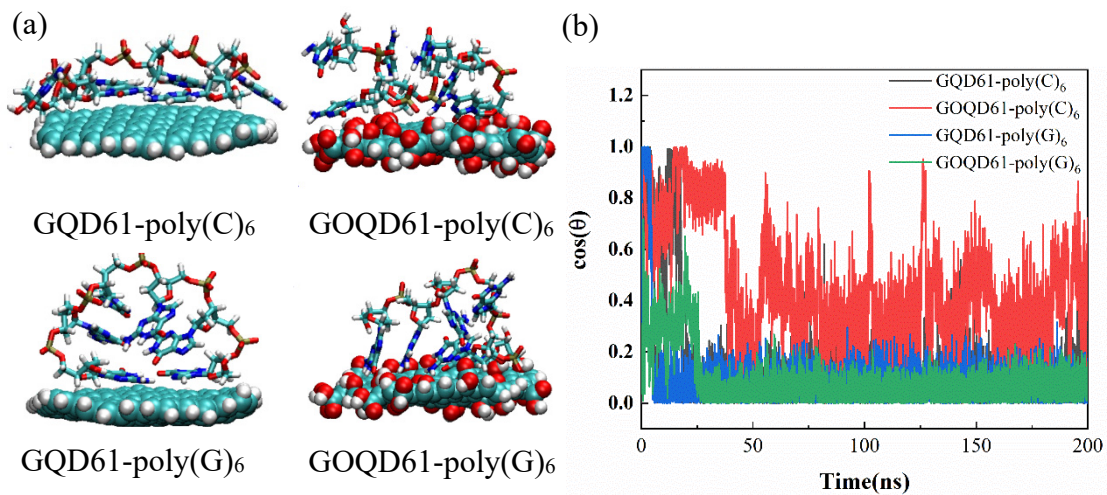


Figure S1. (a) The snapshot of ssDNA adsorbed on the surface of GQD61 and GOQD61 at the end of 200 ns MD simulation; (b) The angle between ssDNA axis and the normal of the GQD61 (GOQD61) surface as a function of simulation time.

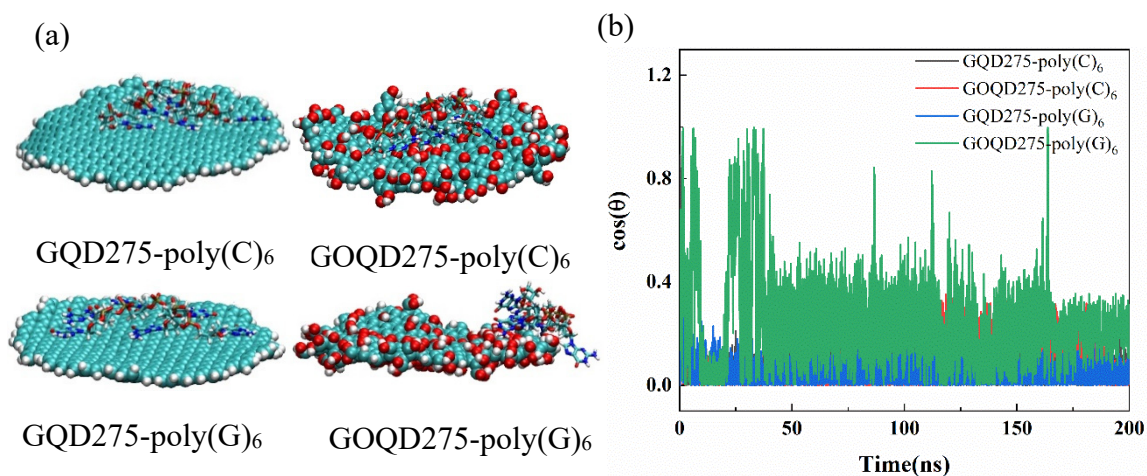


Figure S2. (a) The snapshot of ssDNA adsorbed on the surface of GQD275/GOQD275 at the end of 200 ns MD simulation; (b) The angle between ssDNA axis and the normal of GQD275/GOQD275 surface as a function of simulation time.

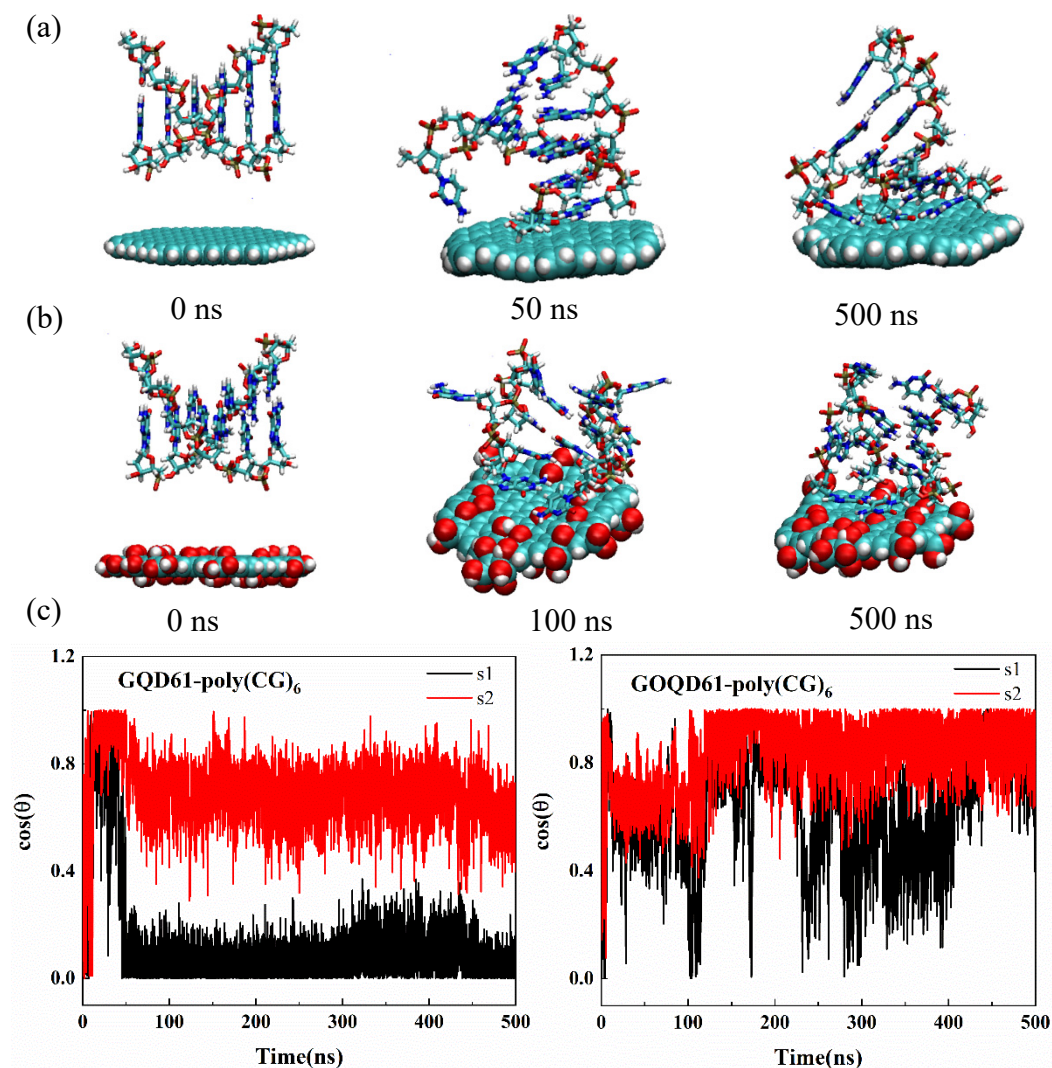


Figure S3. (a) The snapshot of dsDNA adsorbed on the surface of GQD61; (b) The snapshot of dsDNA adsorbed on the surface of GOQD61; (c) The angle between the axis of two single strands of dsDNA and the normal of the GQD61/GOQD61 surface as a function of simulation time.

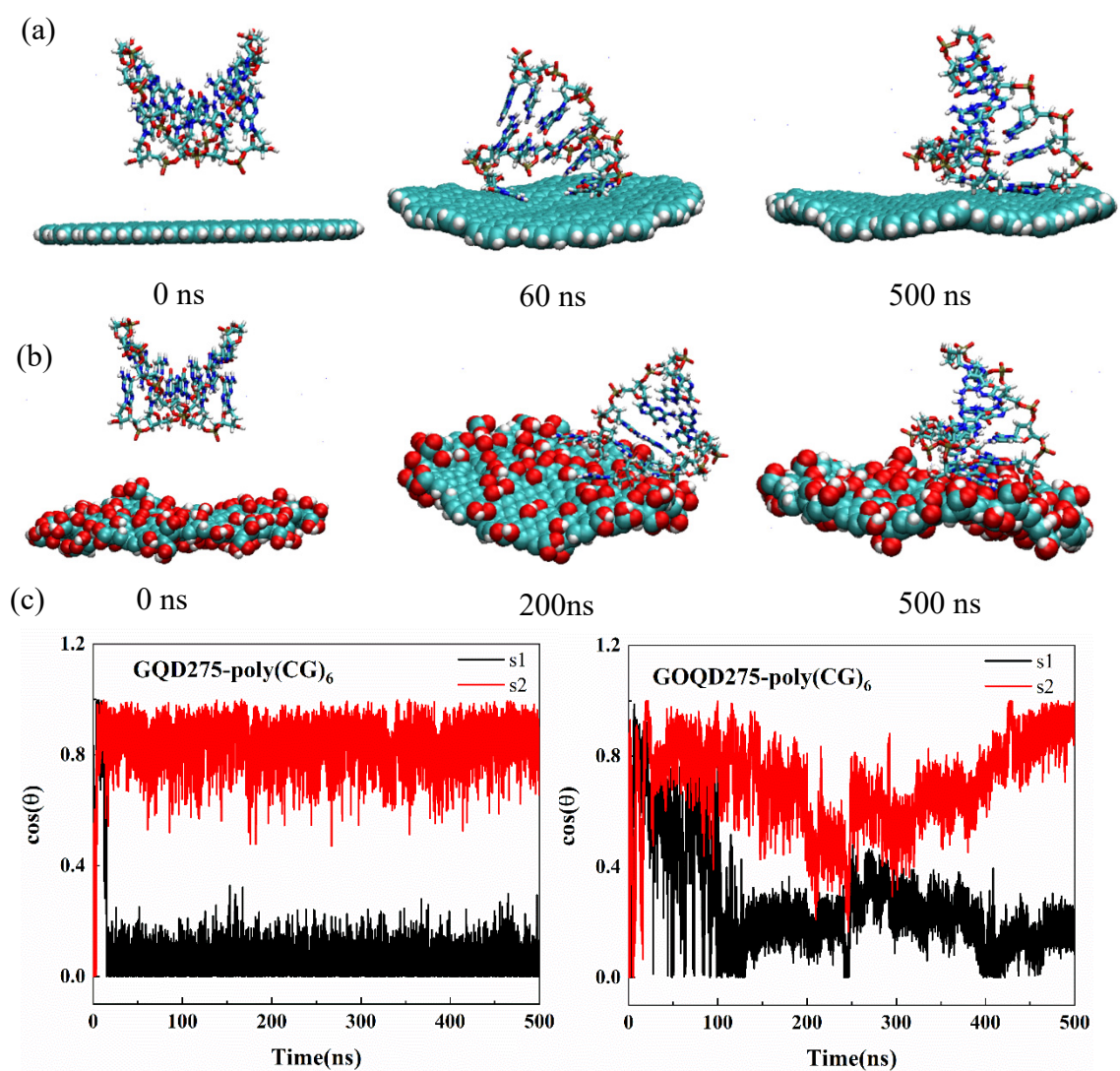


Figure S4. (a) The snapshot of dsDNA adsorbed on the surface of GQD275; (b) The snapshot of dsDNA adsorbed on the surface of GOQD275; (c) The angle between the axis of two single strands of dsDNA and the normal of the GQD275/GOQD275 surface as a function of simulation time.

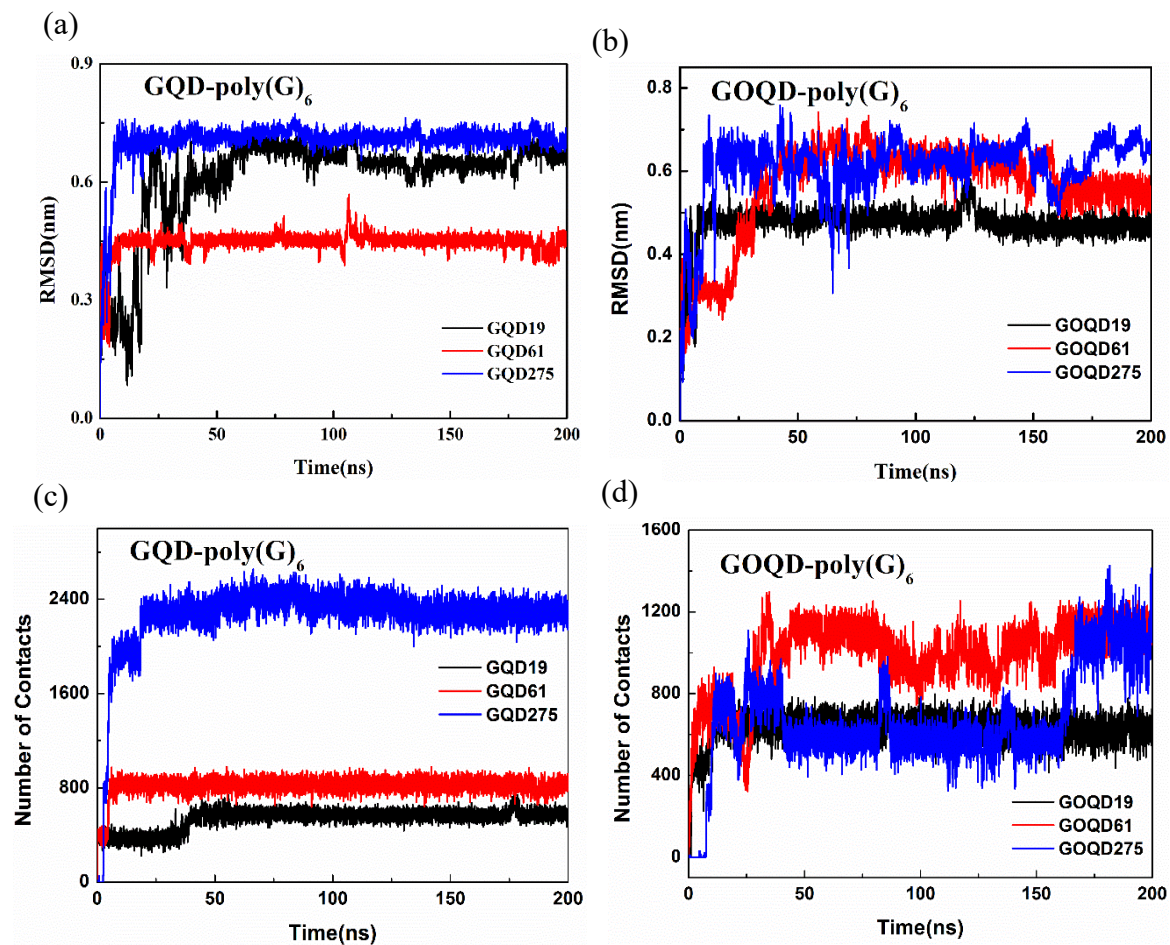


Figure S5. (a) The RMSD variation of poly(G)₆ during the adsorption process on GQD with different sizes; (b) The RMSD variation of poly(G)₆ during the adsorption process on GOQD with different sizes; (c) Number of contacts between poly(G)₆ and GQD versus the simulation time; (d) Number of contacts between poly(G)₆ and GOQD versus the simulation time.

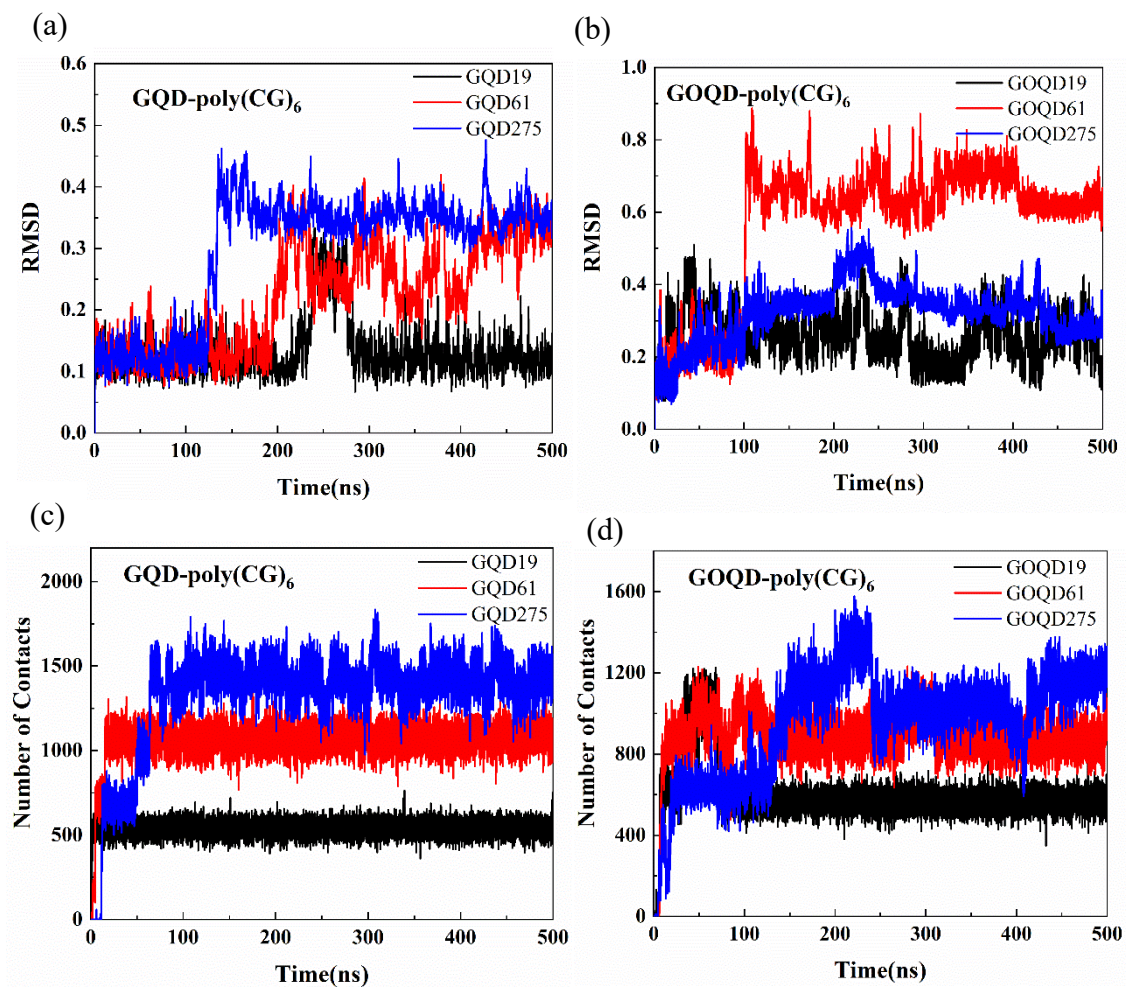


Figure S6. (a) The RMSD during the adsorption of dsDNA on the surface of GQD; (b) The RMSD during the adsorption of dsDNA on the surface of GOQD; (c) Number of contacts between dsDNA and GQD versus the simulation time; (d) Number of contact between dsDNA and GOQD versus the simulation time.