membranes

MDPI

Supplementary Materials

Molecular Dynamics Simulation of Transport Mechanism of Graphene Quantum Dots Through Different Cell Membranes

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Table S1. Details of simulation calculations.

System	No. of atoms	No. of water molecules	Simulation method	GQD:lipid	Time (ns)
GQDs-POPC	117,653	26,939	MD	1:274	200
GQDs-DOPE	126,576	29,624	MD	1:316	200
GQDs-POPE	129,756	27,902	MD	1:342	200
GQDs-POPE-LD	138669	31933	MD	1:342	200
GQDs-POPC	117,653	26,939	SMD	1:274	10
GQDs-DOPE	126,576	29,624	SMD	1:316	10
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GQDs-POPC	117,653	26,939	PMF	1:274	S*10
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GQDs-POPE-LD	138669	31933	PMF	1:342	S*10

MD Simulation

MD simulations were performed using Gromacs5.0 software [1]. The charge of the carbon atom at the edge of GQDs was set to +1.15e; the charge of the hydrogen atom connected to the carbon atom was set to -1.15e, and the remaining carbon atom charge was considered neutral [2]. The relevant parameters of GQDs, including the harmonic bond potentials of C-C and C-H, the harmonic angles of C-C-H and C-C-C, the harmonic dihedral potential, and Lennard-Jones (LJ), were taken from ref [3]. LJ and charge parameters are listed in Table 2.These parameters have been successfully used to explore the interaction between GQDs and DNA, and the transmembrane transport of GQDs [2,4–7]. All systems were subjected to 50,000 steps of energy minimization and 1 ns pre-equilibration before the MD simulation. All bond lengths and all angles involving hydrogen atoms were constrained using the LINCS algorithm. The NPT ensemble was used in the simulation with a constant temperature of 314 K imposed by a Berensdsen thermostat and 1 bar of pressure controlled by a semi-isotropic Parrinello–Rahman barostat. The cutoff for the nonbonded van der Waals interaction was set by a switching function starting at 1.0 nm and reaching zero at 1.2 nm. The long-range electrostatic interaction was calculated by particle mesh Ewald (PME) summation, with a cutoff of 1.2 nm for the separation of the direct and reciprocal space summation.

Table S2. The LJ and charge parameters used in the MD

Element	C(sp2)	C_{CH}	H_{CH}
ε (kcal/mol)	0.0859	0.046	0.0301
σ (Å)	3.3997	2.985	2.42
q(e)	0	−0.115	0.115
Reference	[8]	[9]	[9]

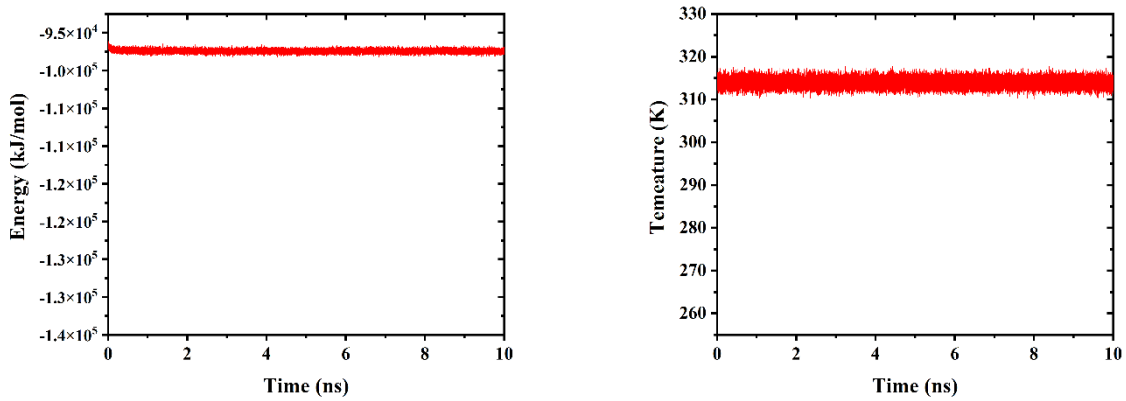

Figure S1. Changes in energy and temperature of the system.

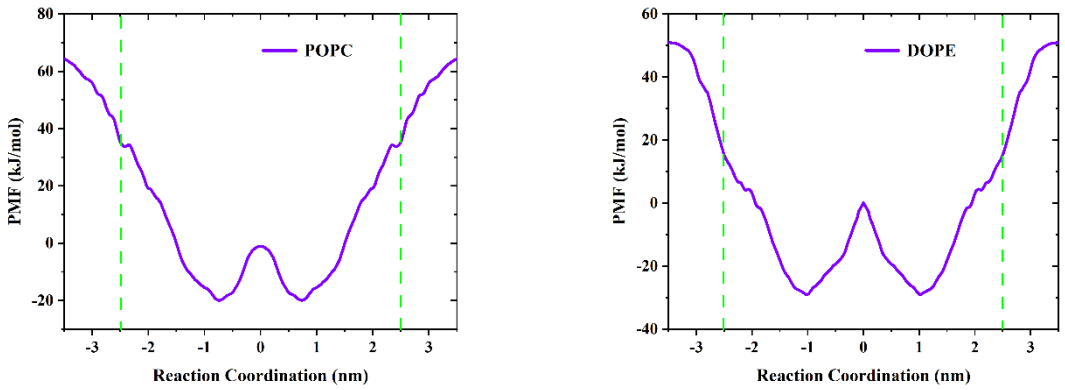

Figure S2. The average force (PMF) potential of GQDs transport through the membrane. The green dotted line indicates the two boundaries of the cell membrane.

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