Supplementary Information

Role of electrostatic potential polarization in the translocation of graphene quantum dots across membranes

Xiaofeng Tang, [†,±] Shitong Zhang,[†,±] Hong Zhou,[†] Bo Zhou,[‡] Shengtang Liu,[*,†] Zaixing Yang,[*,†]

[†]*Institute of Quantitative Biology and Medicine, State Key Laboratory of Radiation Medicine and Protection, School of Radiation Medicine and Protection, Collaborative Innovation Center of Radiological Medicine of Jiangsu Higher Education Institutions, Soochow University, Jiangsu 215123, China.*

[‡]*School of Electronic Engineering, Chengdu Technological University, Chengdu 611730, China*

[±] These authors contributed equally.

Corresponding Author

Prof. Zaixing Yang (zxyang@suda.edu.cn), Dr. Shengtang Liu (liushengtang@suda.edu.cn)

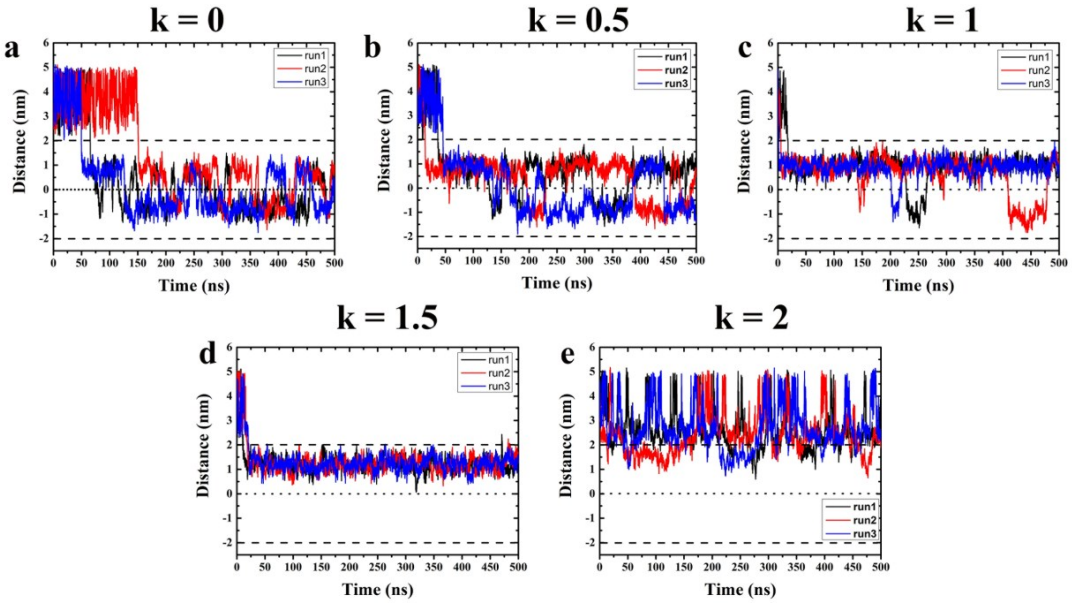

Figure S1. Time evolution of the distance of the center of mass (COM) between GQD and POPC membrane along *z*-axis with different k: (a) $k = 0$, (b) $k = 0.5$, (c) $k = 1$, (d) $k = 1.5$, (e) $k = 2$, for three independent trajectories. The dashed lines represented the location of the top end (2 nm), and bottom end (-2 nm) of the POPC membrane, the dots line (0 nm) represented the middle of the bilayers.

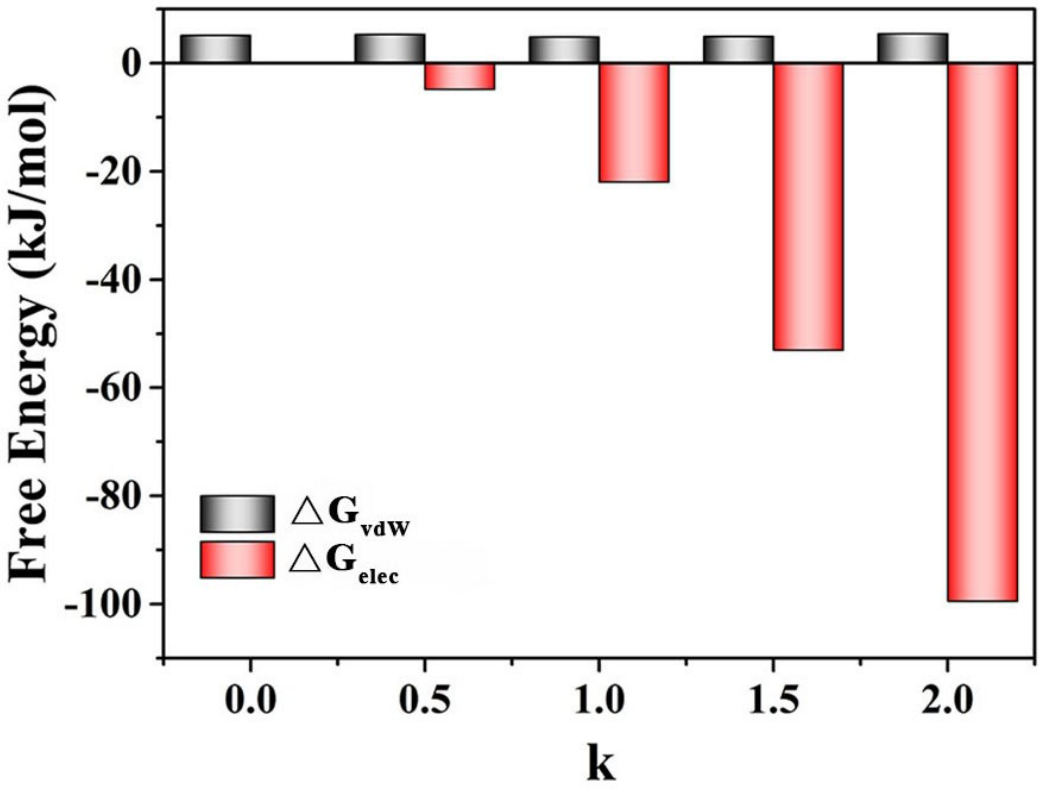

Figure S2. The contribution of Coulomb (black) and van der Waals (red) interactions to hydration of GQDs with different *k*. The 46-window (46 λ points) scheme was adopted for coupling non-bonded interaction, λ = 0.00, 0.001, 0.01, 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.35, 0.40, 0.45, 0.50, 0.55, 0.60, 0.65, 0.70, 0.75, 0.80, 0.85, 0.90, 0.95, 0.99, 0.999, 1.00 for turn on the vdW interaction, and λ = 0.00, 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.35, 0.40, 0.45, 0.50, 0.55, 0.60, 0.65, 0.70, 0.75, 0.80, 0.85, 0.90, 0.95, 1.00 for turn on the electrostatic interaction, respectively.

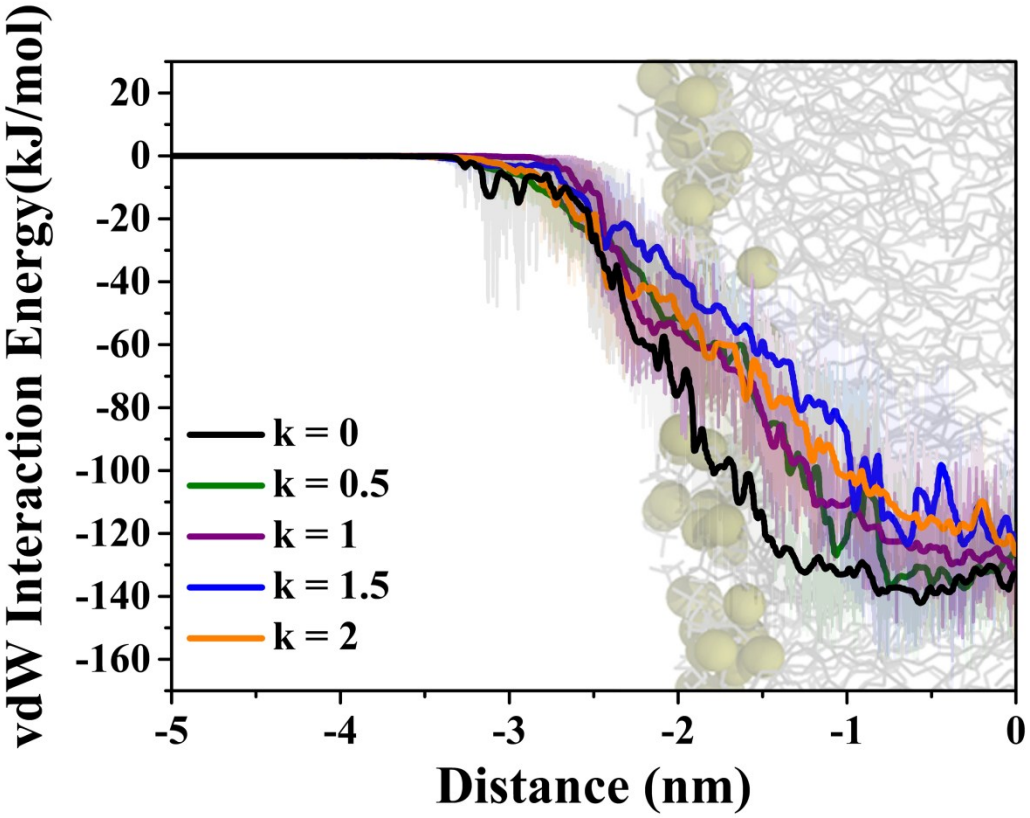

Figure S3. Van der Waals interactions between GQDs and POPC membrane with different *k*. The black, olive, purple, blue and orange line represented *k* = 0.0, 0.5, 1.0, 1.5 and 2.0, respectively.