

Electronic Supporting Information for:

Accelerated evaporation of water on Graphene Oxide

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Content

Water evaporation on homogeneous GO and patterned GO with SPC/E water model

The surface tension of TIP3P water model is 52.3 mJ/m² at 300K, while the surface tension of SPC/E water model is 63.6 mJ/m² at 300K [J. Chem. Phys. 126, 154707]. In order to test the influence of water model with different interfacial tension, we have tried the simulation of water evaporation with water model of SPC/E.

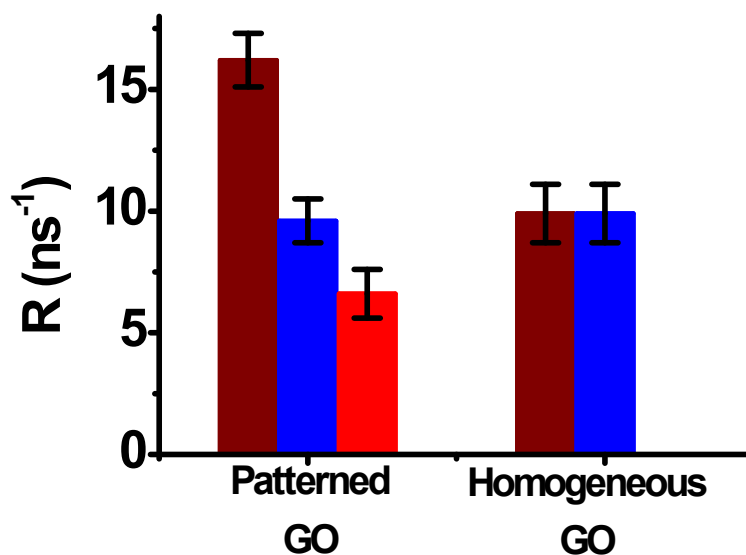


Fig.S11 Evaporation of 9102 SPC/E water molecules on homogeneous GO and patterned GO surface. The brown, blue, and red solid columns represent the total evaporation rate R_{total} , the evaporation rate $R_{oxidized}$ from the oxidized region, and the evaporation rate $R_{unoxidized}$ from the unoxidized region on the homogeneous and patterned GO, respectively.

We have performed new molecular dynamics (MD) simulations on the evaporation of SPC/E water molecules on homogeneous GO and patterned GO surface. As shown in Fig. SI1, for SPC/E water model, R_{total} for the patterned GO (16.2 ns^{-1}) is also much larger than R_{total} on the homogeneous GO (9.9 ns^{-1}). This accelerated evaporation of water on the patterned GO surface can also be attributed to the slightly decreased $R_{oxidized}$ of 9.6 nm^{-1} and the considerable $R_{unoxidized}$ of 6.6 nm^{-1} . Although the value of evaporation rate is different with different water models, the enhancement of water evaporation on the patterned GO surface and the mechanism behind such phenomena still remain.