Electronic Supplementary Information

Molecular Dynamics Simulations of Hyperbranched Poly(ethylene imine) – Graphene Oxide Nanocomposites as Dye Adsorbents for Water Purification

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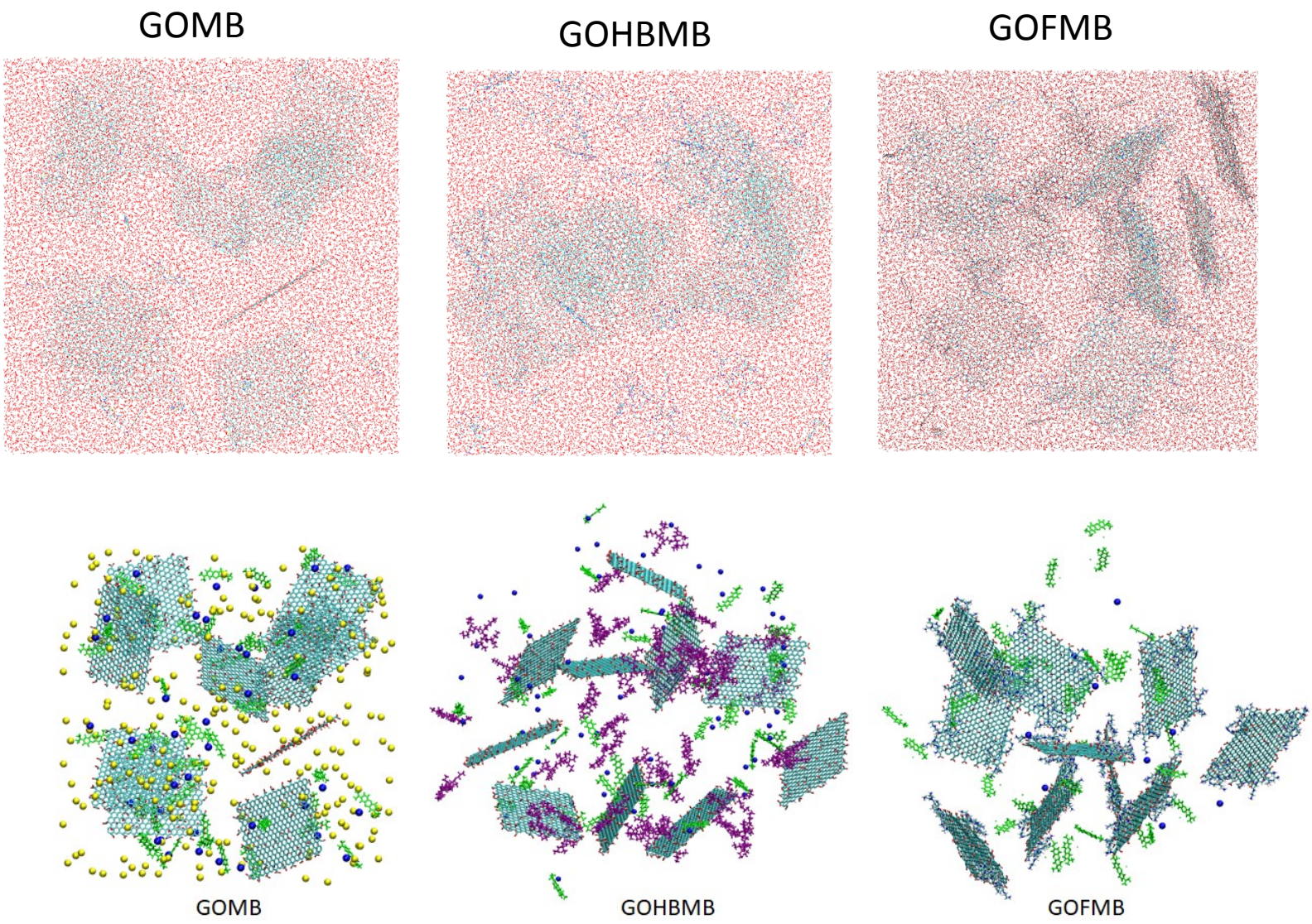


Figure S1. Snapshots of the initial configurations of the systems including water molecules (upper row) and with the water molecules removed (lower row) for better visualization. Hydrogen and oxygen atoms are shown as white and red dots, respectively. The color code for the GO flakes is the same as that described in figure 1 of the main text. Chlorine and Sodium counterions are shown as blue and yellow spheres respectively, MB molecules are shown in green and free BPEI polymers are portrayed in purple.

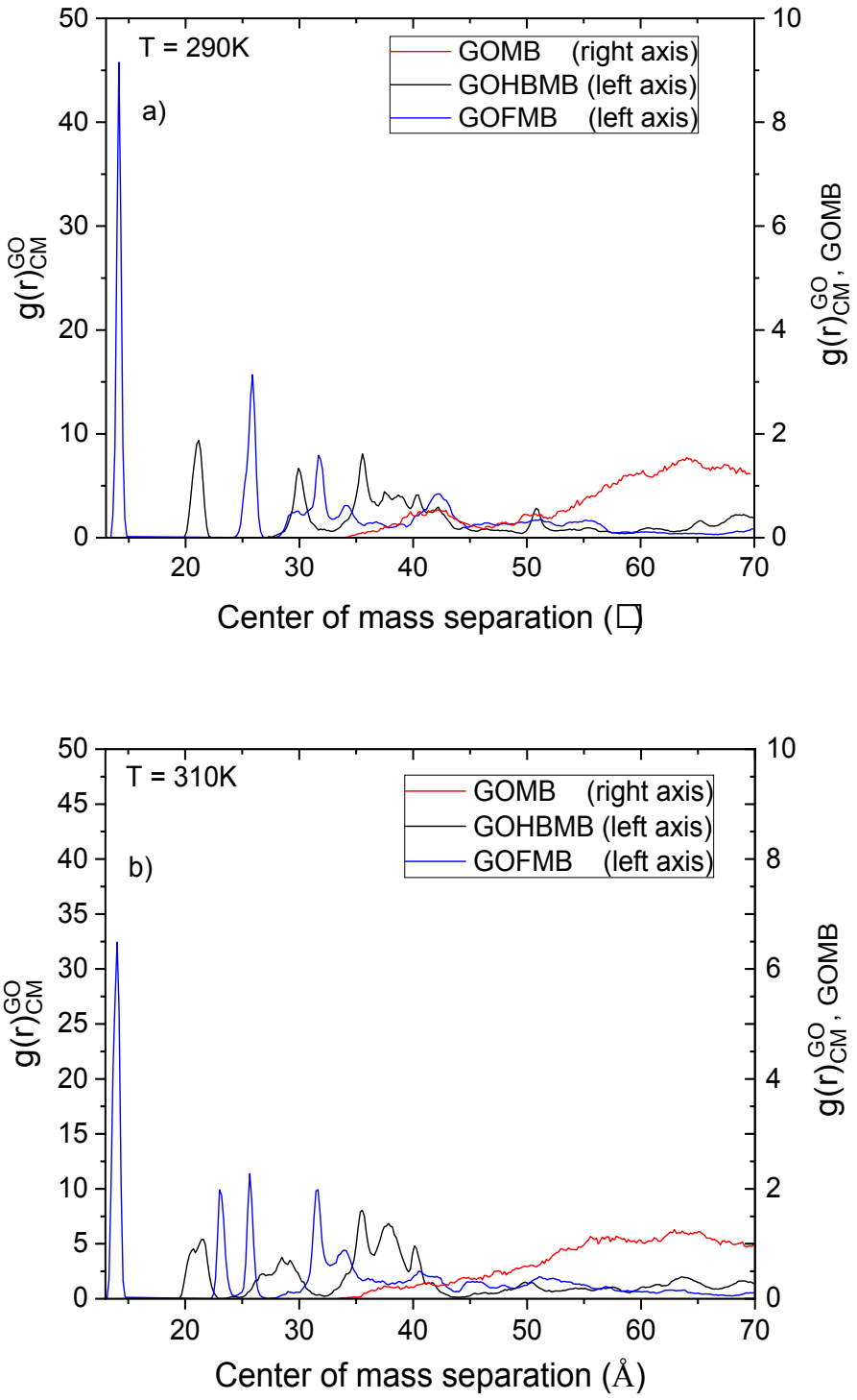


Figure S2. Radial distribution functions arising from the centers of mass of the GO flakes at a)$T = 290$K and β) at $T = 310$K, in the GOMB, the GOHBMB and the GOFMB models.

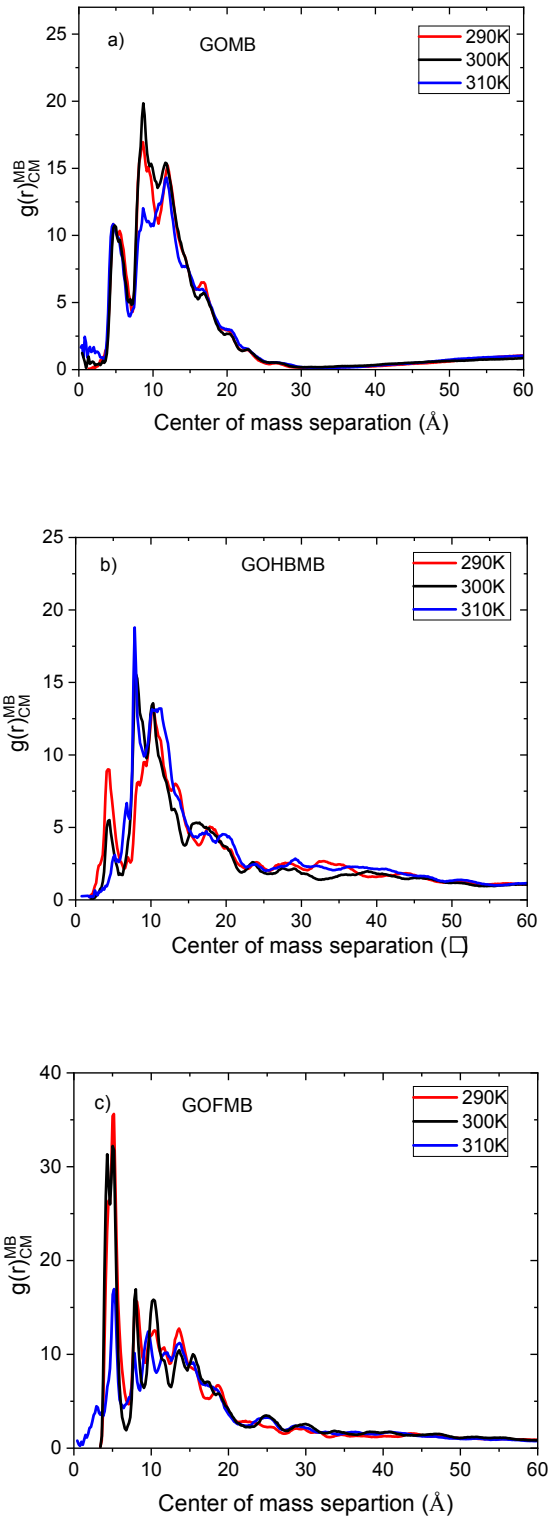


Figure S3. Radial distribution functions arising from the centers of mass of the MB molecules in a) the GOMB, b) the GOHBMB and c) the GOFMB models, at T=290, 300 and 310K.

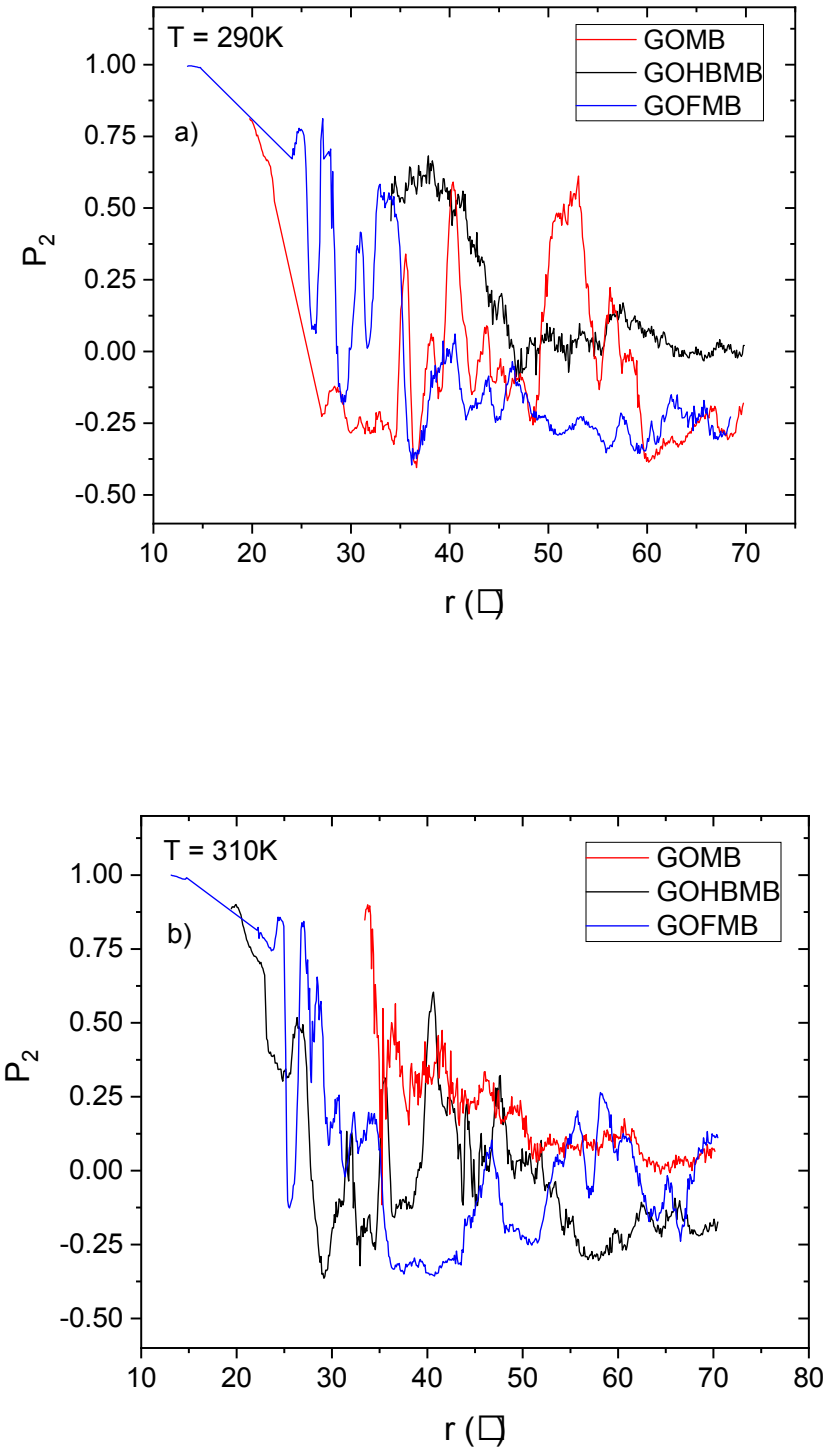
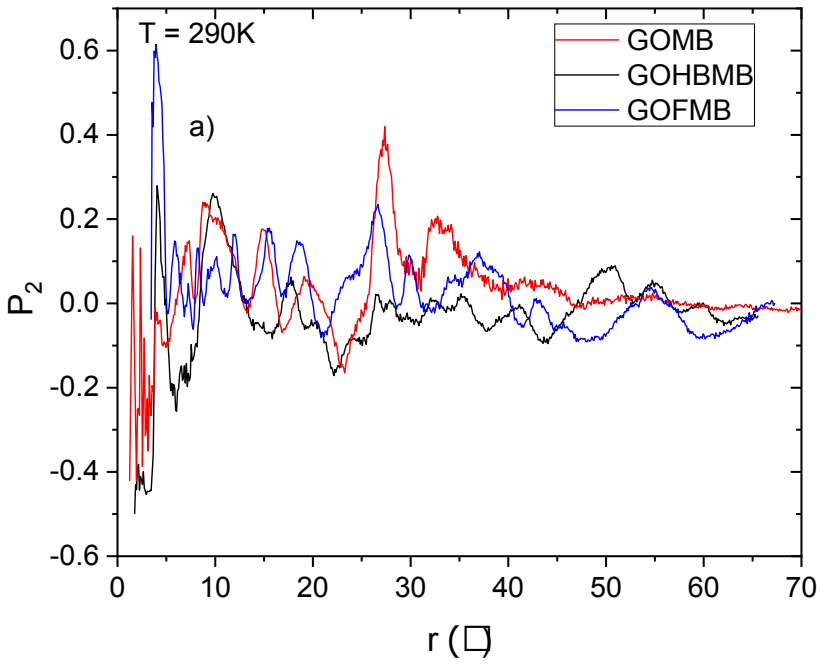


Figure S4. Orientational order parameter (see text) of the GO flakes in the GOMB, the GOHBMB and the GOFMB models, as a function of the center of mass separation between two molecules, at a) T=290K and at b) T = 310K.



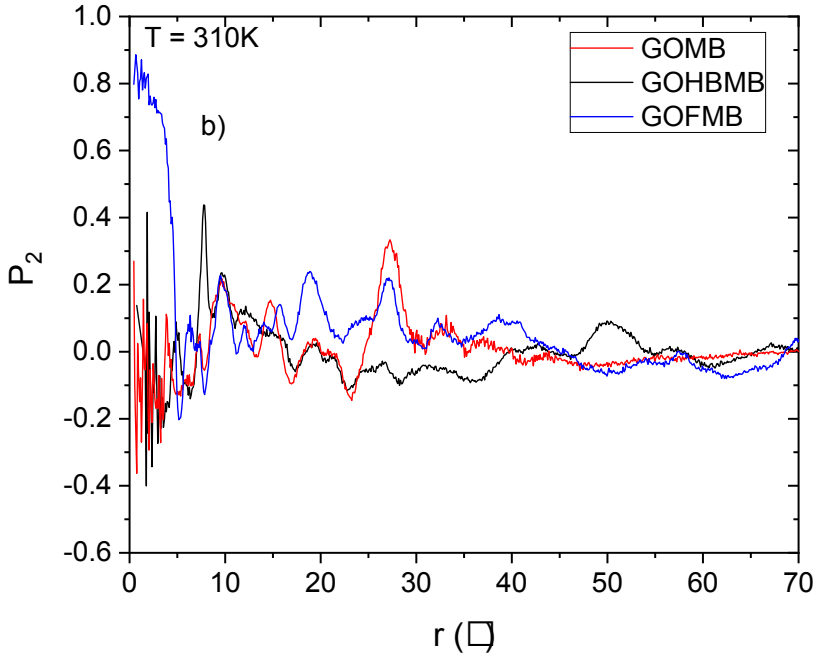
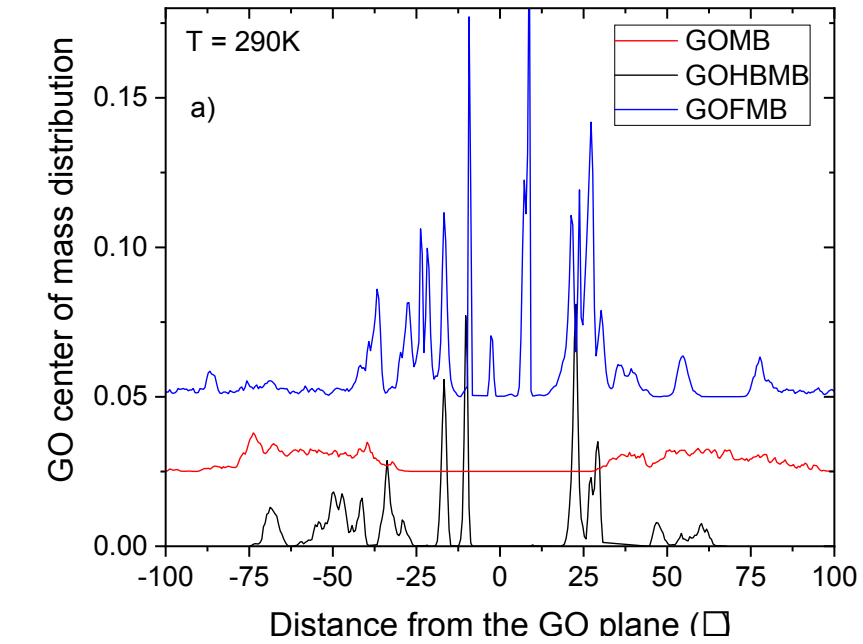


Figure S5. Orientational order parameter (see text) of the MB molecules in the GOMB, the GOHBMB and the GOFMB models, as a function of the center of mass separation between two molecules, at a) $T = 290$K and at b) $T = 310$K.



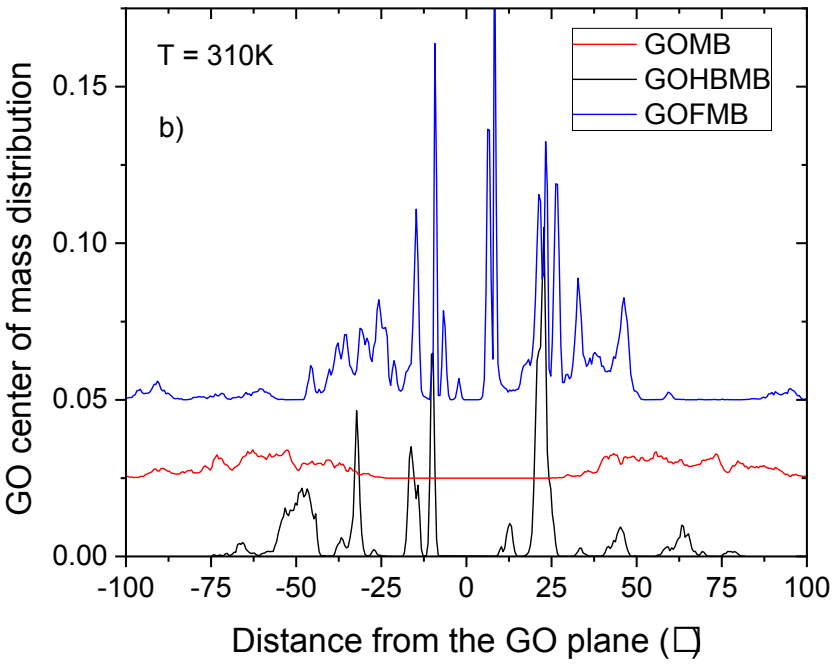
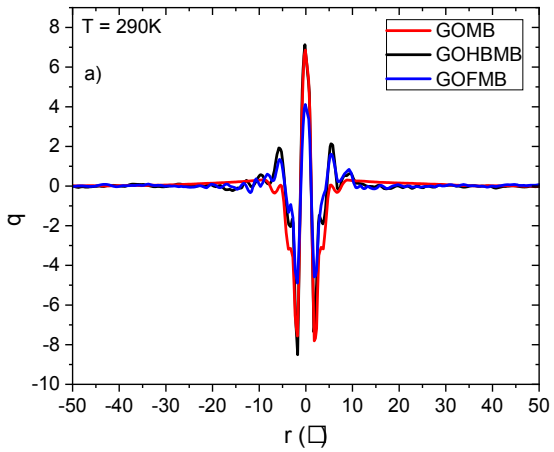
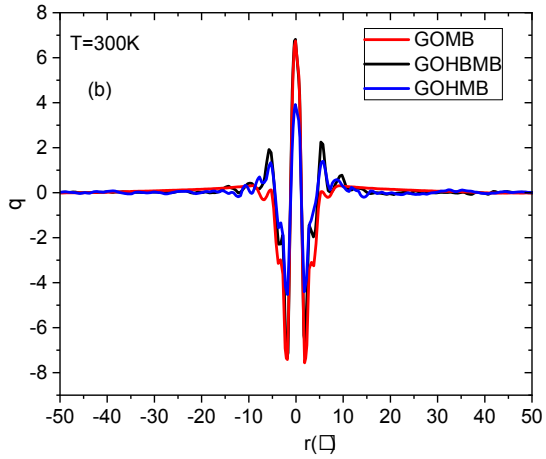


Figure S6. Center of mass distribution profiles of the GO molecules in a direction normal to the GO plane, for the GOMB, GOHBMB and GOFMB models, at a) T = 290 K and b) T = 310K. Distance 0 denotes the position of the GO plane. Positive and negative coordinates correspond to placements of the molecules on the right and on the left side of the plane of the reference GO molecule. respectively. The spectra of GOMB and GOFMB are shifted by 0.025 and 0.05 respectively, in the y-axis for clarity





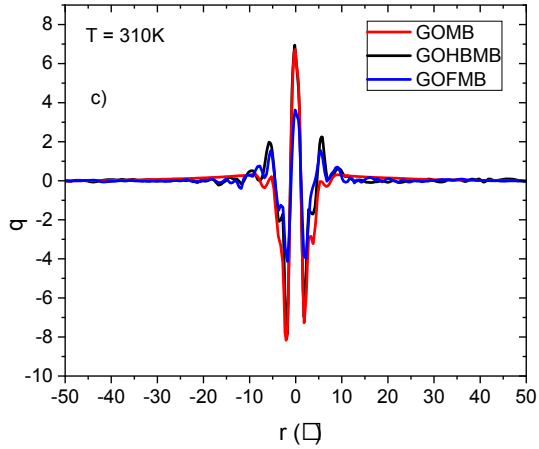
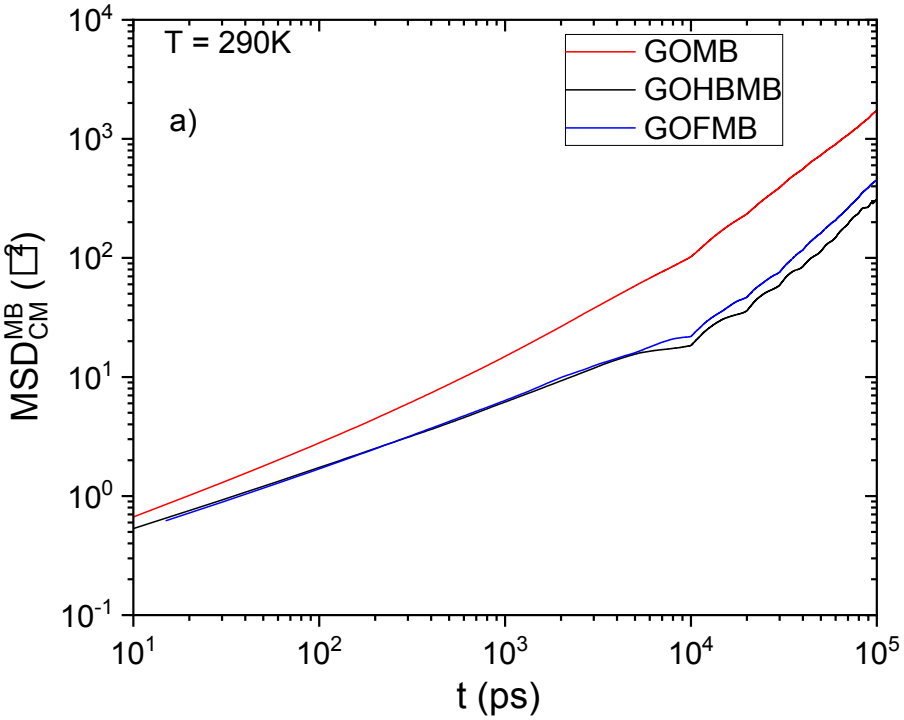


Figure S7. Charge distributions (electron charge units) along a direction normal to the GO plane arising from the charged moieties at a) T = 290K b) T=300K and c) T = 310K, for the GOMB, GOHBMB and the GOFMB systems. Distance r=0 denotes the location of the GO plane.



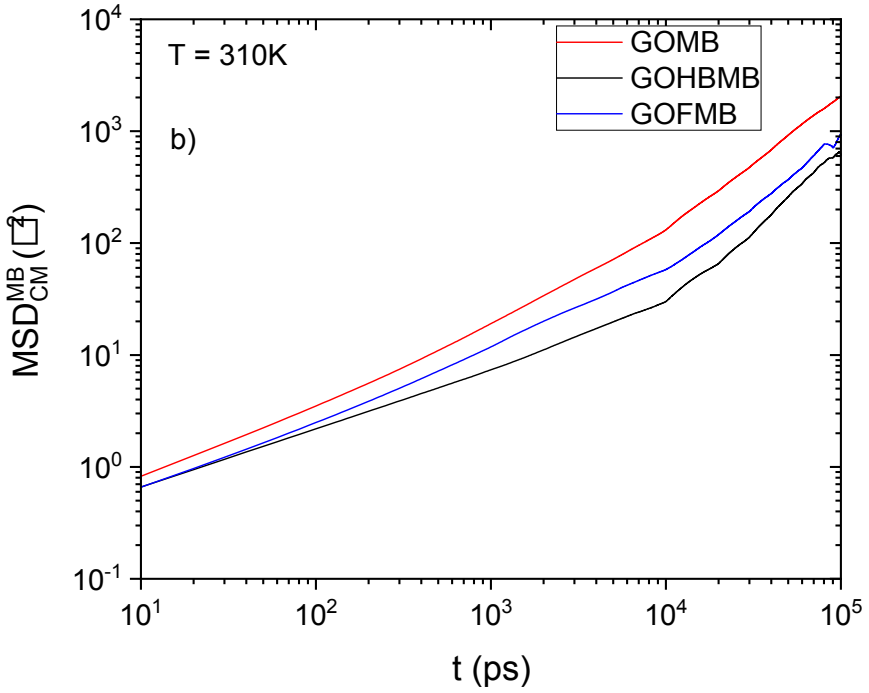


Figure S8. Mean Squared Displacement (MSD) of the centers of mass of the dye molecules at a) $T = 290$K and b) $T = 310$K.

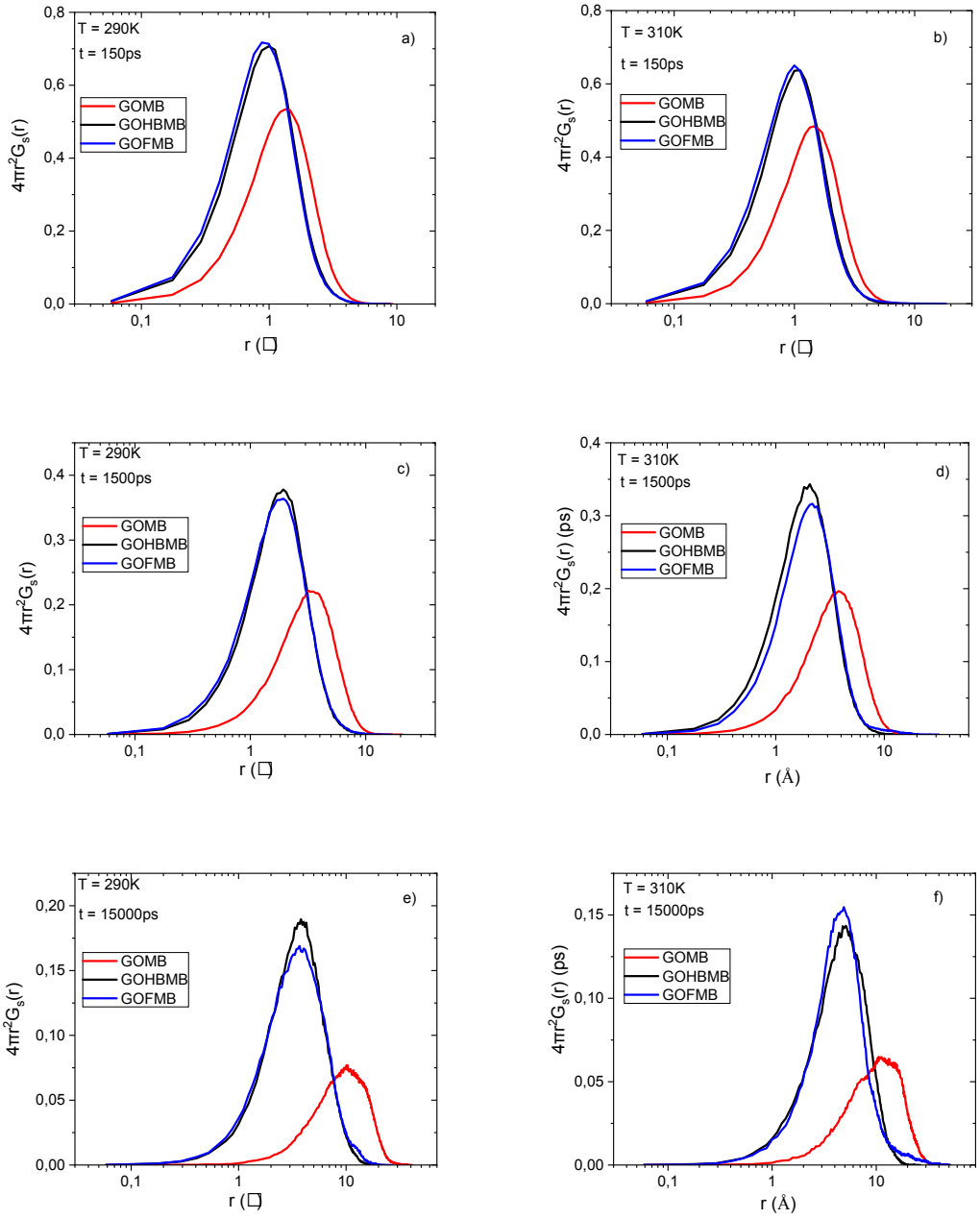
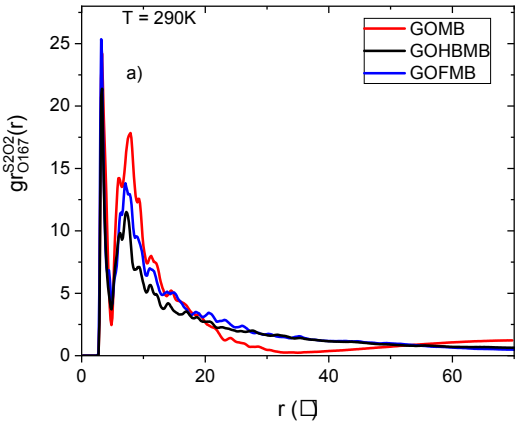
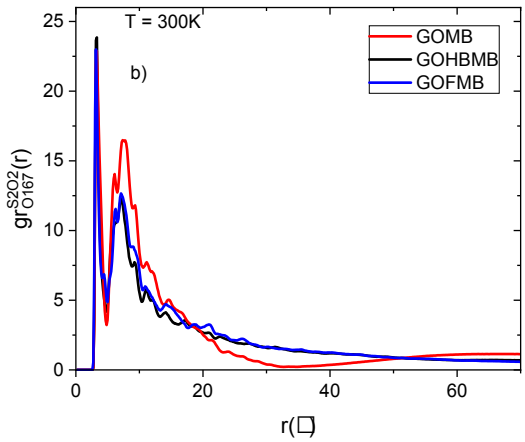


Figure S9. Comparison of the self van Hove functions (multiplied by $4\pi r^2$) describing the MBs' motion in all systems at temperatures and times a) T = 290K, t = 150ps, b) T = 310K, t = 150ps, c) T = 290K, t = 1500ps, d) T = 310K, t = 1500ps, e) T = 290K, t = 15000ps and f) T = 290K, t = 15000ps





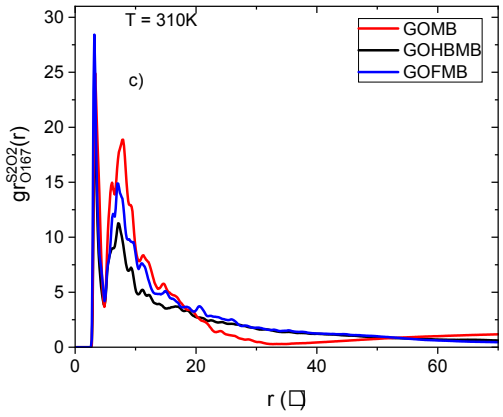


Figure S10. Sulfur (MB) – hydroxyl oxygen (GO) radial distribution functions for all the examined models at a) T = 290K, b) T = 300K and c) T = 310K

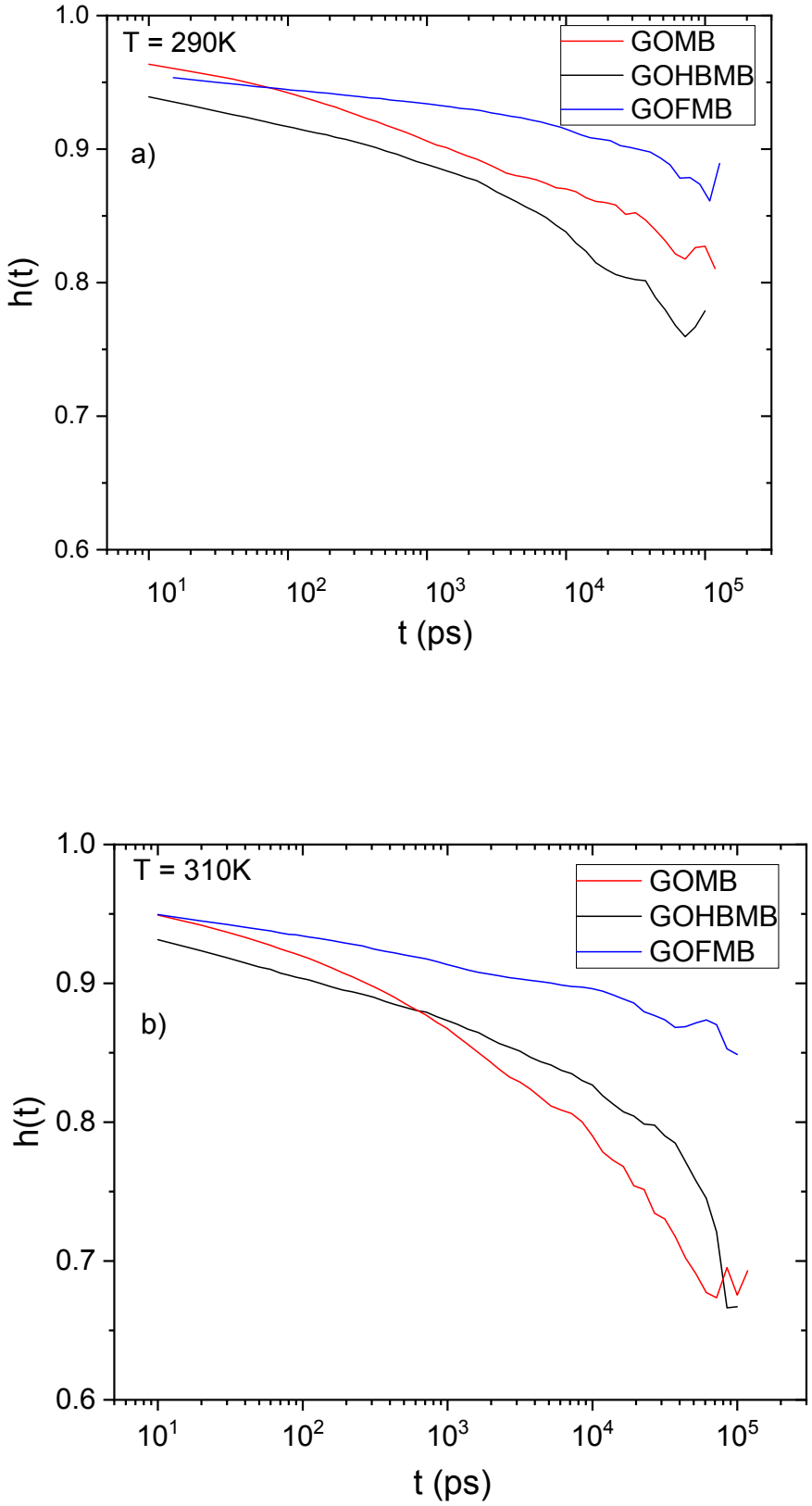


Figure S11. Sulfur (MB) – hydroxyl oxygen (GO) pair correlation functions at a) T = 290K and b) T = 310K, for all the examined models.