ELECTRONIC SUPPLEMENTARY INFORMATION

Dispersion of Non-Covalently Modified Graphene in Aqueous Medium: A Molecular Dynamics Simulation Approach

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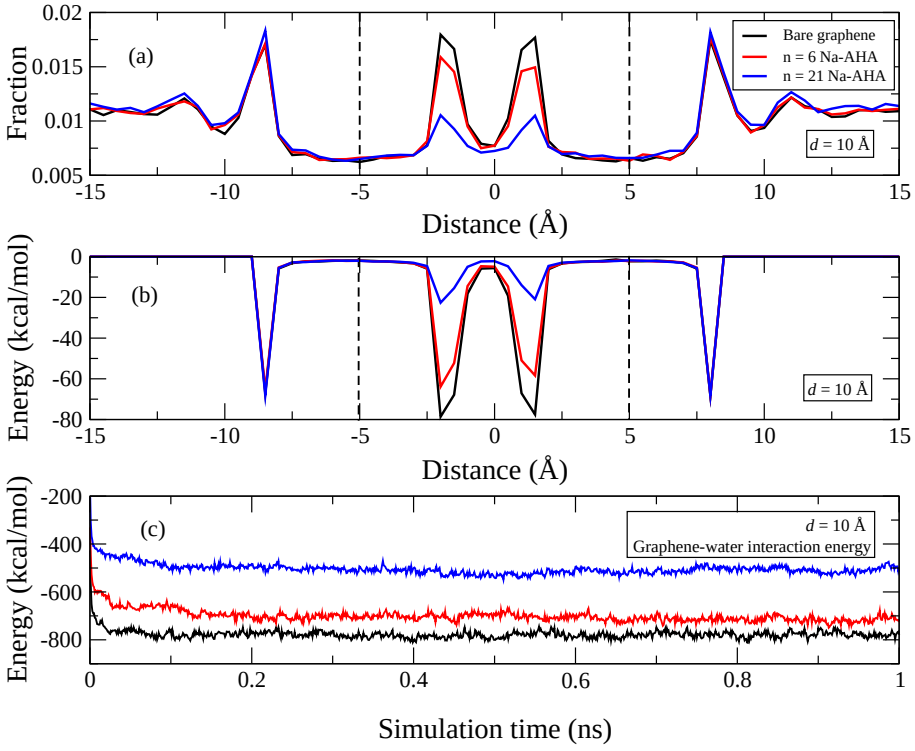

FIG. S1: (a)Plot of fractional number density of water molecules in the simulation box along the X-axis (separation axis) for $d = 10$ Å. (b) Direct calcualtion of the variation of graphene-water interaction energy as a function of the x for the range -8.5 $\leq x \leq$ 8.5 showing that the graphene-water interaction energy progressively becomes less negative with increasing n. (c) Time-series plot of the overall graphene-water interaction energy for different n showing an increase in graphene-water interaction energy with corresponding increase in n. The vertical dashed lines indicate the location of the two graphene sheets in the simulation box for the corresponding separation distances in (a) – (c). The different concentrations are represented by the colors, black ($n = 0$), red ($n = 6$), and blue ($n = 21$) for all plots (a) – (c).

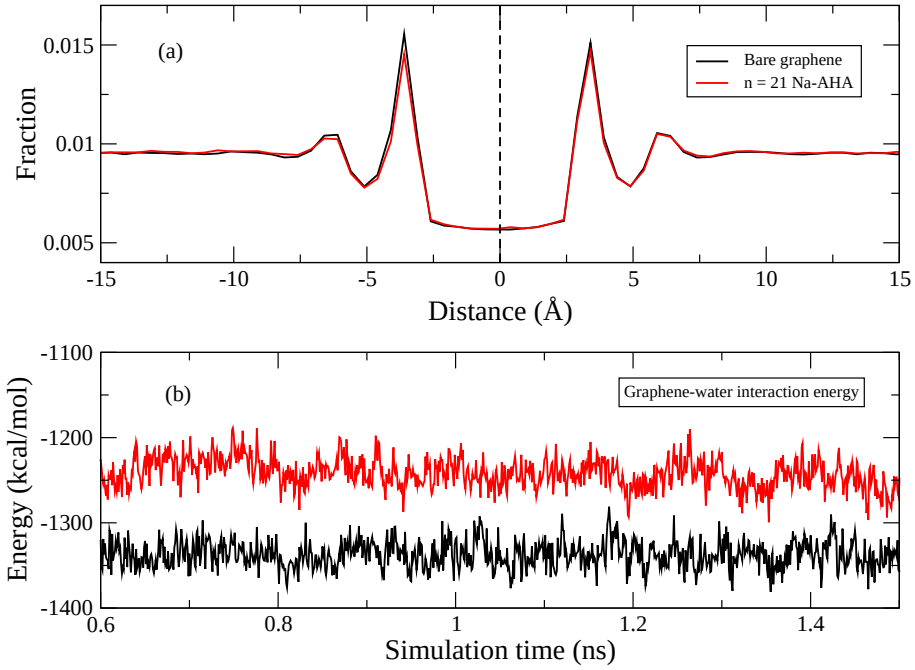

FIG. S2: (a)Plot of fractional number density of water molecules in the simulation box along the X-axis (separation axis) in contact with a single graphene of area 50 $\times$ 50 Å^2. (b) Time-series plot of the overall graphene-water interaction energy for different $n = 0$ and $n = 21$ showing that the graphene-water interaction energy is less negative for $n = 21$. The different concentrations are represented by the colors, black ($n = 0$) and red ($n = 21$) for plots (a) and (b).