Supplementary Information

for

Poly(Vinyl Alcohol) as a Water Protecting Agent for a Silver Nanoparticle: A Role of Polymer Size and Structure

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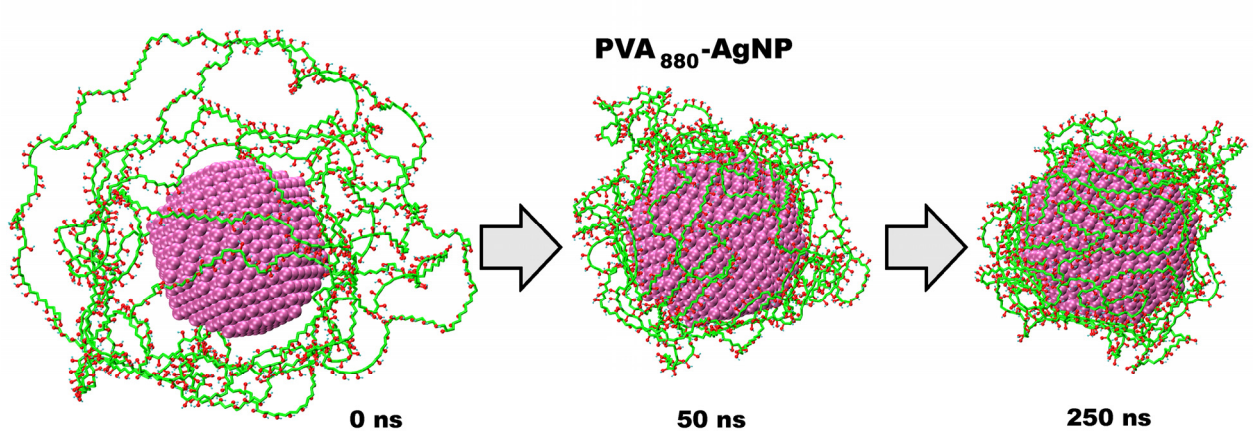
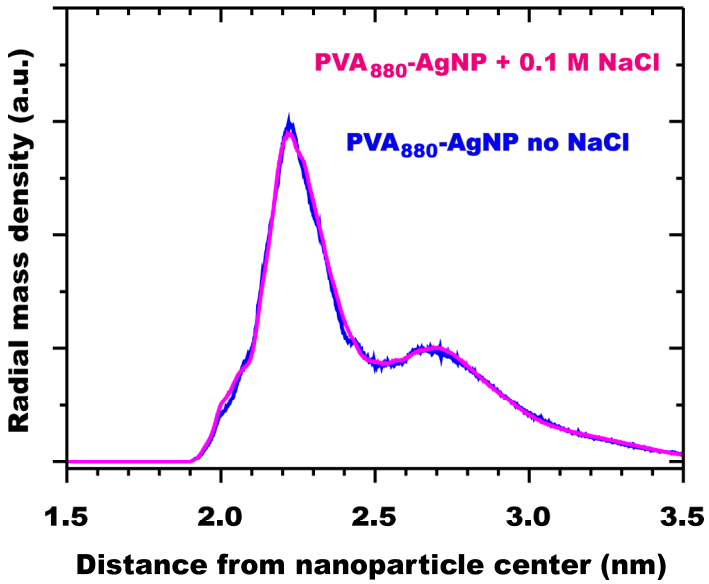
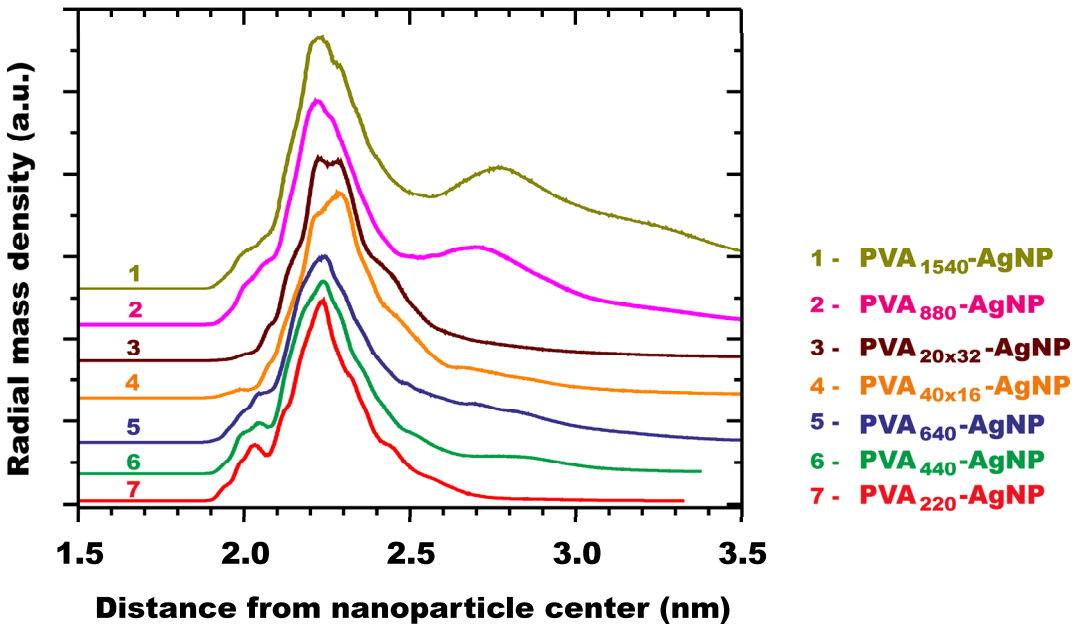


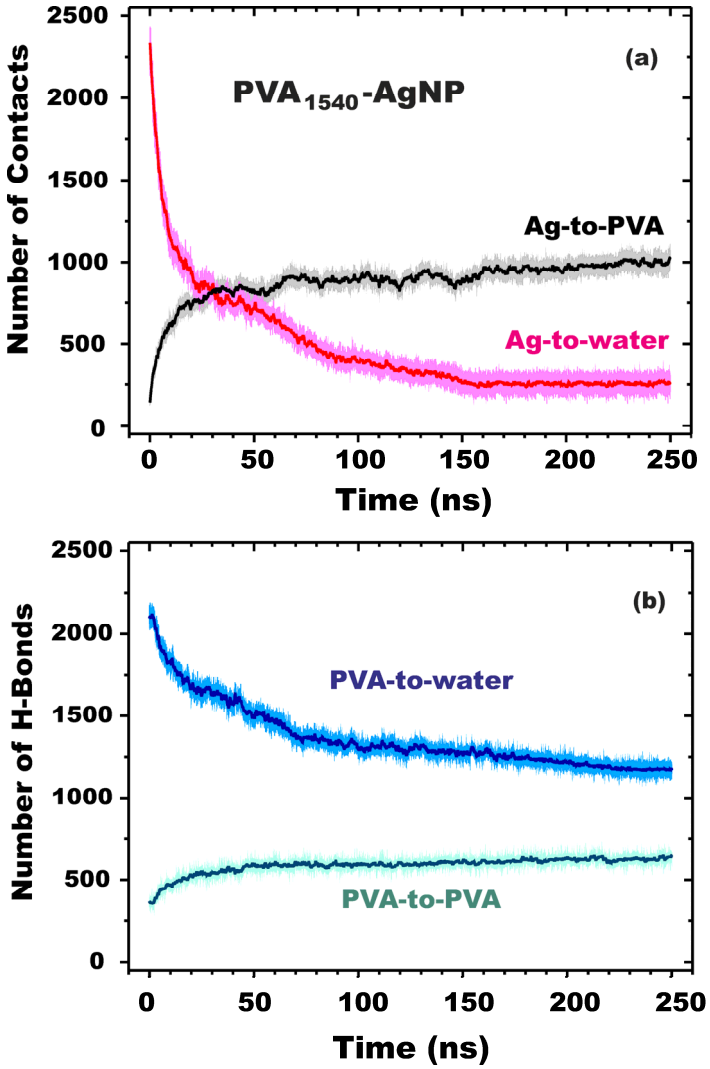
Supplemental Figure S01. MD simulations of PVA$_{880}$−AgNP. Adsorption dynamics of PVA$_{880}$ onto AgNP core was simulated at the NPT ensemble. The silver atoms are shown by the van der Waals model colored in *mauve*. PVA backbone is shown in *green*. The PVA oxygen atoms are *red* balls. Water molecules and buffering ions are not shown for clarity.



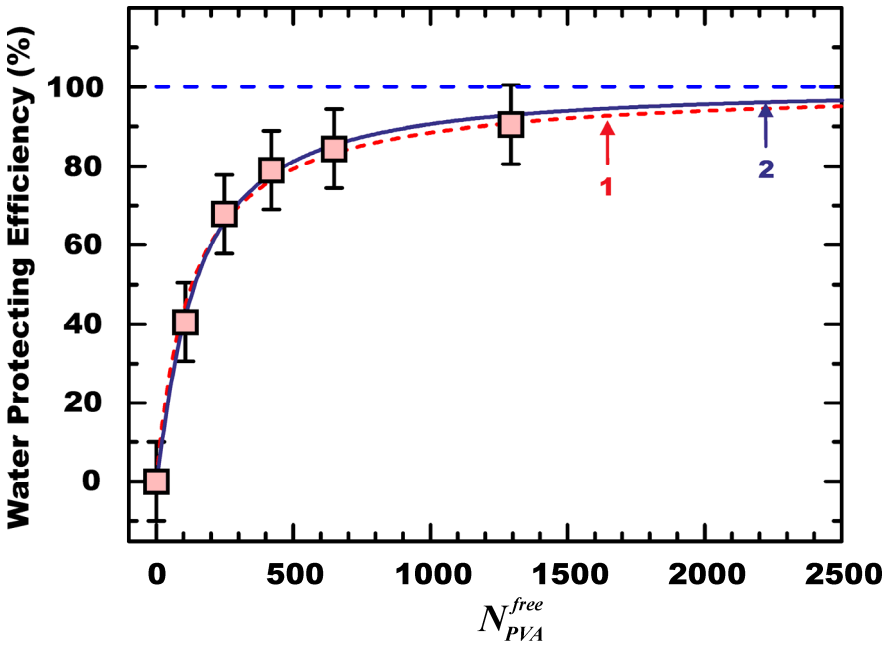
Supplemental Figure S02. Radial distribution functions calculated from the center-of-mass (RDF-COM) of the inorganic Ag core. The RDF-COM profiles for PVA in the absence (*blue*) and in the presence of 0.1 M buffering ions NaCl (*magenta*) reveal the similar pattern.



Supplemental Figure S03. Radial distribution functions calculated from the center-of-mass (RDF-COM) of the inorganic Ag core. The RDF-COM profiles for PVA with the different polymer size and structure show the gradual formation of multilayered coating around the Ag core upon going from PVA_{220} up to PVA_{1540}.



Supplemental Figure S04. (***a***) Time evolution of the number of contacts between the Ag atoms and all the PVA atoms (Ag-to-PVA), and the oxygen atoms of the water molecules (Ag-to-water) calculated for PVA_{1540}-AgNP with the cut-off 3.5 Å. (***b***) Dynamics of the number of hydrogen bonds (PVA-to-water and PVA-to-PVA) calculated for PVA_{1540}-AgNP.



Supplemental Figure S05. Water-protecting effect of PVA. Plots of the water-protecting efficiency of PVA (*squares*) for AgNP as a function of the free unbound number of PVA units estimated by the MD simulation. The data are fitted by (*1*) Langmuir-type (K=7.68·10^{-3}, W_{max}=3200) and (*2*) Langmuir−Freundlich-type (K=3.26·10^{-3}, n=0.86, W_{max}=2800) adsorption isotherms.