Supplementary Information:

Microstructure-related performances of poly(vinyl alcohol)-silica hybrid membranes: A molecular dynamics simulation study

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Table of figures

Part. A **Flow charts for studying PVA membrane and its hybrid membranes by MD simulations**

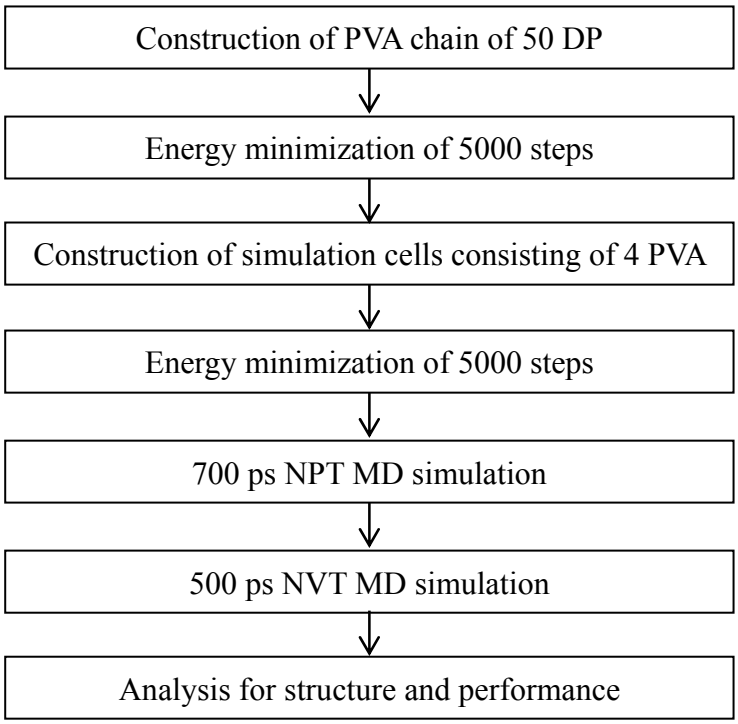

Fig. S1 Flow chart for studying PVA membrane by MD simulations.

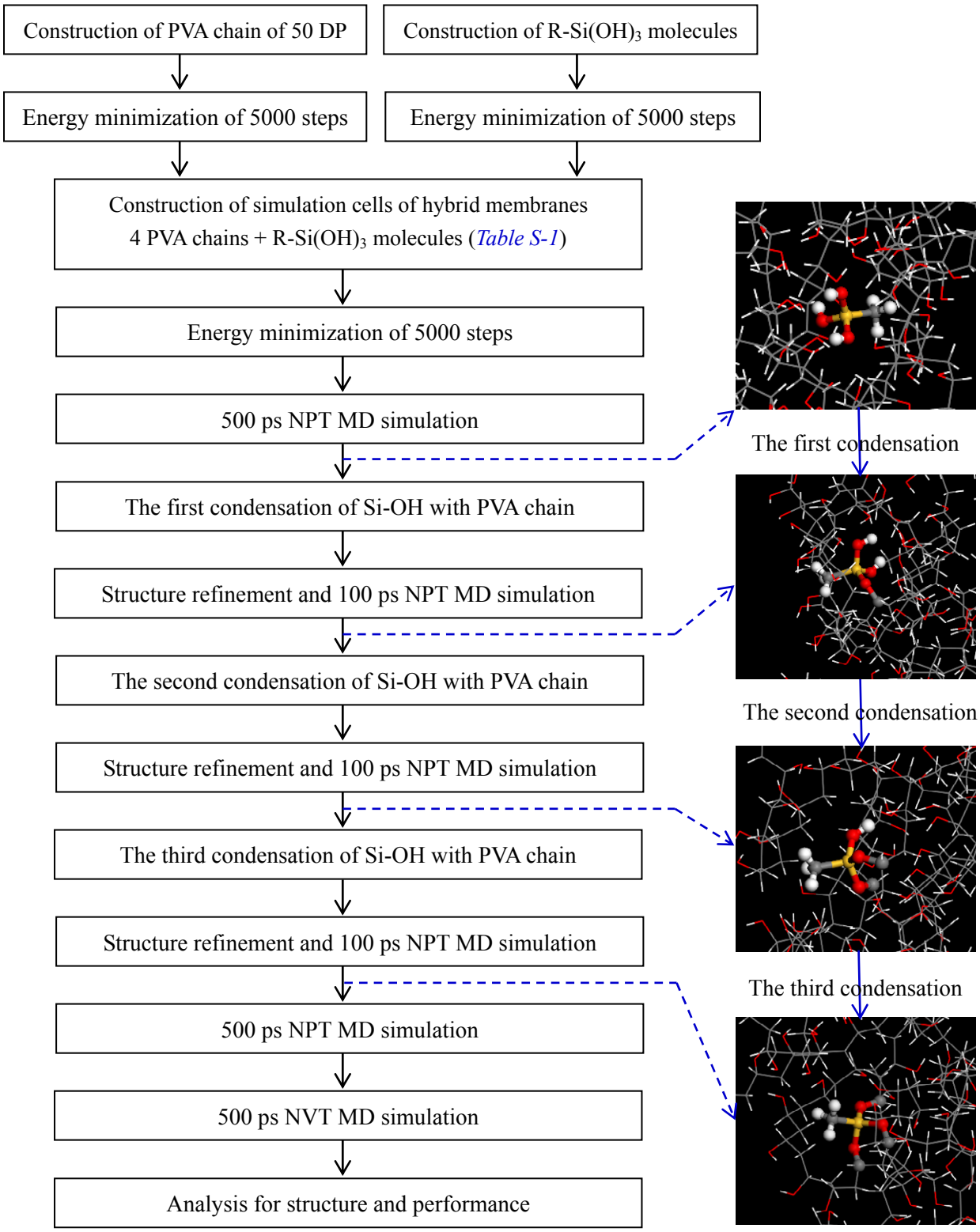

Fig. S2 Flow chart for studying PVA-silica hybrid membrane by MD simulations.

***Part. B* Solubility parameters of the PVA-silica hybrid membranes**

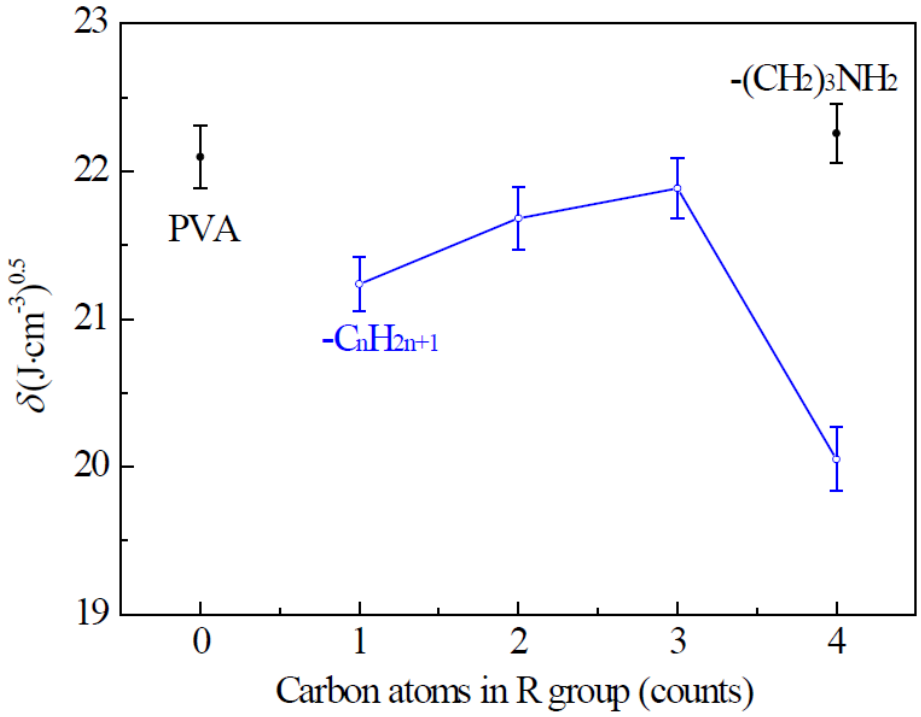

Fig.S3 Solubility parameters of the PVA-silica hybrid membranes.

***Part. C* Effect of APTS content on properties of the PVA/APTS hybrid membranes**

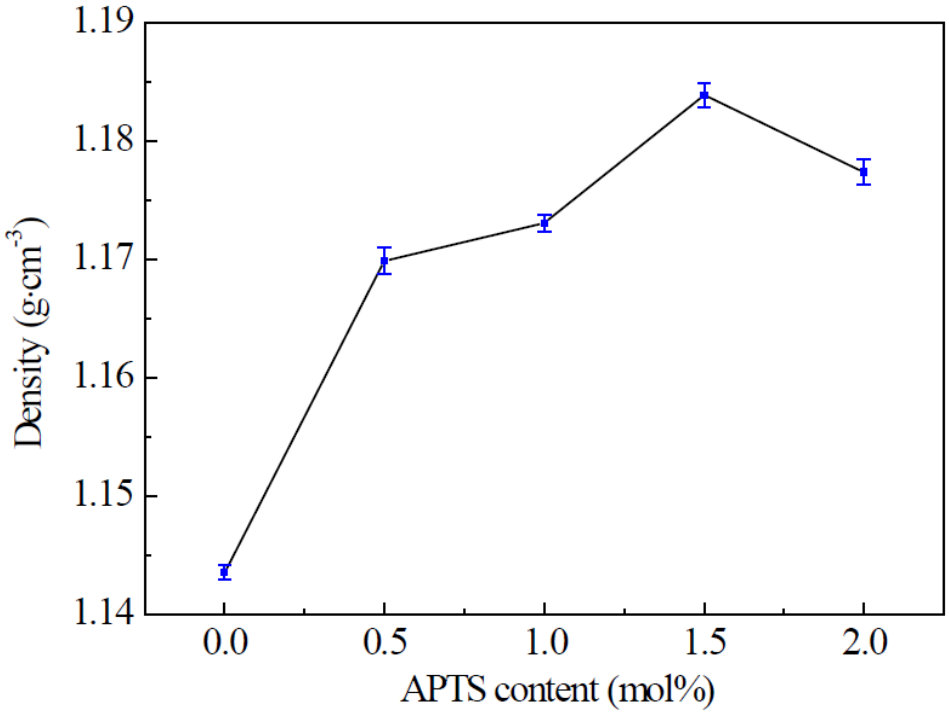

Fig.S4 Effect of APTS content on density of the hybrid membranes.

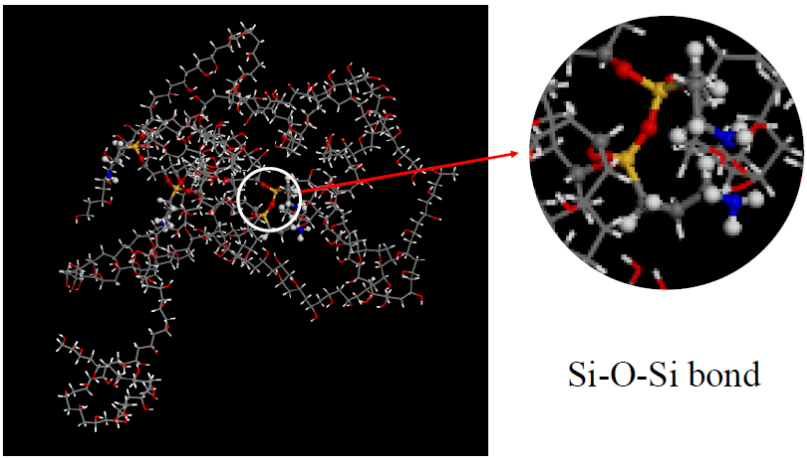

Fig.S5 Chemical structure of self-condensation of APTS in the hybrid membrane with 2 mol% APTS.

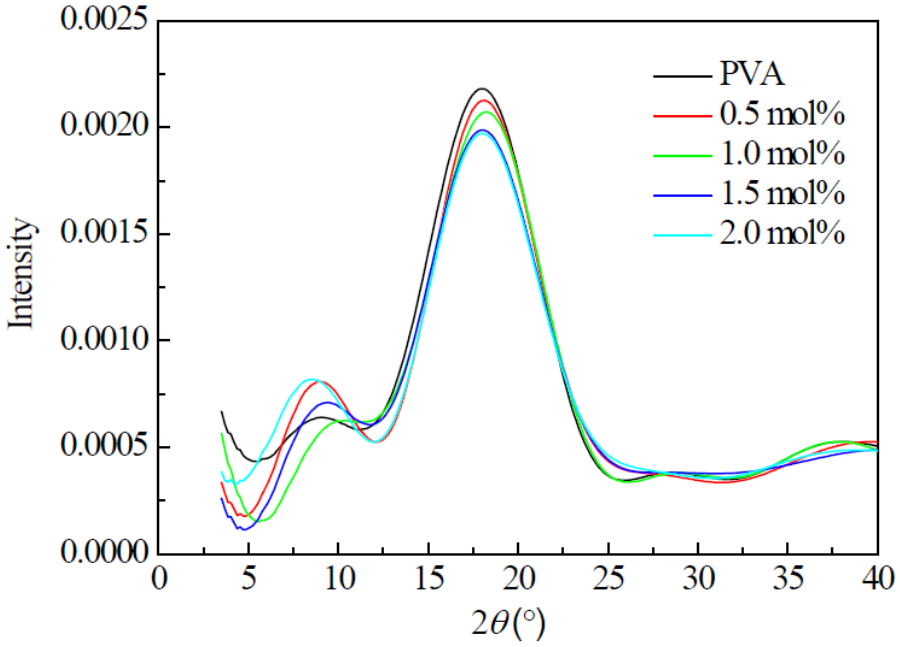

Fig.S6 Effect of APTS content on the simulated X-ray scattering spectra of the hybrid membranes.

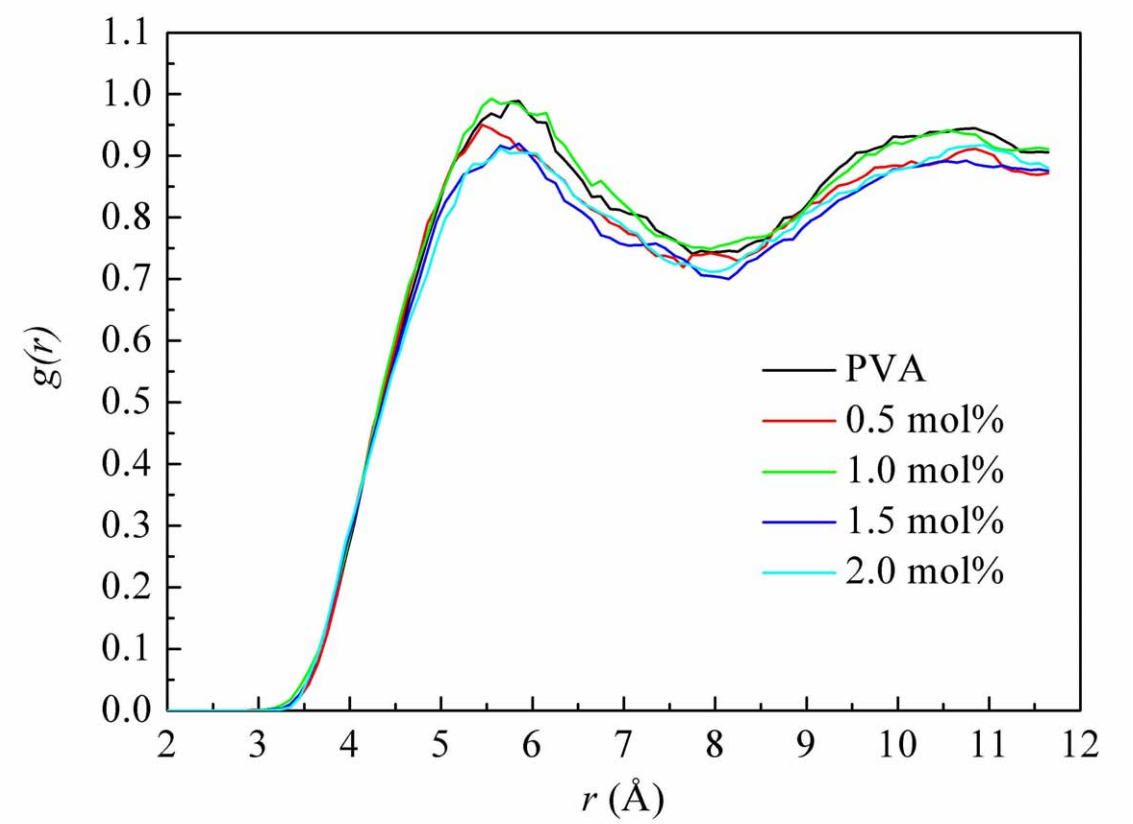

Fig. S7 Effect of APTS content on the interchain (*g(r)*) of backbone carbon atoms from PVA chains in the hybrid membranes.