Electronic Supplementary Material (ESI) for Polymer Chemistry.

Interfacial regions in spherical nanoparticle-doped glassy polymer: Interfaces or interphases?

Jinming Chang[a], Xiaoyu Guan[b], Yi Chen[a,*], Haojun Fan[b]

[a] *National Engineering Laboratory for Clean Technology of Leather Manufacture, Sichuan University, Chengdu, 610065, P.R. China*

[b] *Key Laboratory of Leather Chemistry and Engineering of Ministry of Education, Sichuan University, Chengdu, 610065, P.R. China*

* Corresponding author. Tel.: +86 28 85401068; fax: +86 28 85405237.

E-mail address: chenyi_leon@scu.edu.cn (Y. Chen)

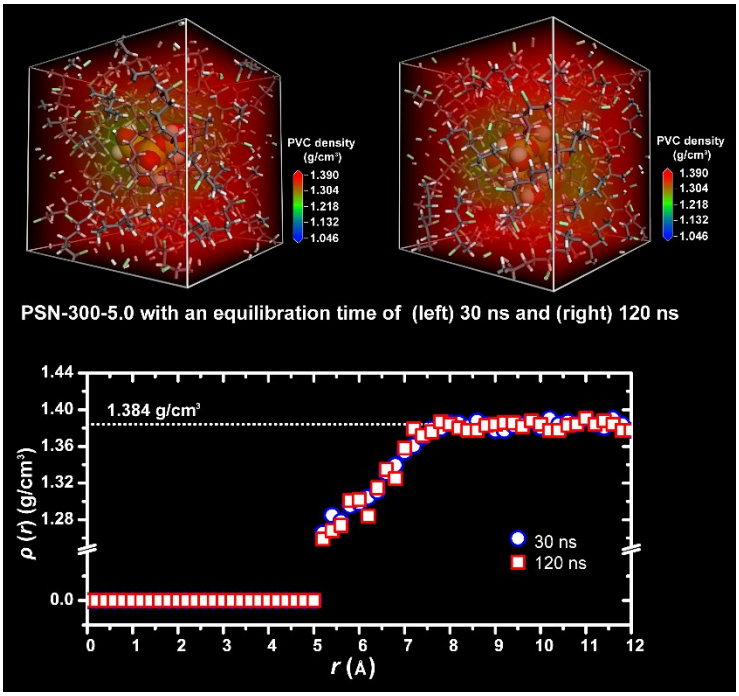

Figure S1. Three-dimensional density field of PVC component in PSN-300-5.0 for different equilibration time, where the PVC chains were displayed as sticks while these atoms constituting the silica (~5.0 Å in radius) were rendered as spheres with radii equivalent to their van der Waals radii. To access the interior view, the density field was generated in transparent mode. Radial density profiles of PVC component as a function of distance from the silica centroid were also present. To ensure an adequate resolution to discern onset of density fluctuation, the space around the silica centroid was divided equally into a sequence of thin concentric spherical shells with an identical thickness of 0.2 Å. The density of PVC component in these shells was then calculated to generate the distribution profiles. A sudden increase in PVC density from zero was

visible that defined periphery of the filler particle. The white dashed line represented the average density of PVC component in undoped controls.