

Supporting Information

for

QM/MD simulations on the role of SiO₂ in polymeric insulation materials

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Figure Caption:

Figure S1. The last snapshots at 60 ps for a-c) Model S_{1-3}^0 ; d-f) Model S_{1-3}^{1-} ; g-i) Model S_{1-3}^{2-} ; j-l)
Model S_{1-3}^{3-} ; m-o) Model S_{1-3}^{4-} ; p-r) Model L_{1-3}^0 ; s-u) Model L_{1-3}^{1-} .

Figure S2. The RDF of Mulliken charge distribution around SiO₂ nanoparticles for each trajectory.
a-e) for Model S^n (n=0-4); f-g) for Model L^n (n=0, 1).

Figure S3. The Lindman Index (L.I.) a, b) of C and all atoms for PE, S^n , L^n (n=0, 1); c, d) of C and all
atoms for S^n (n=0-4).

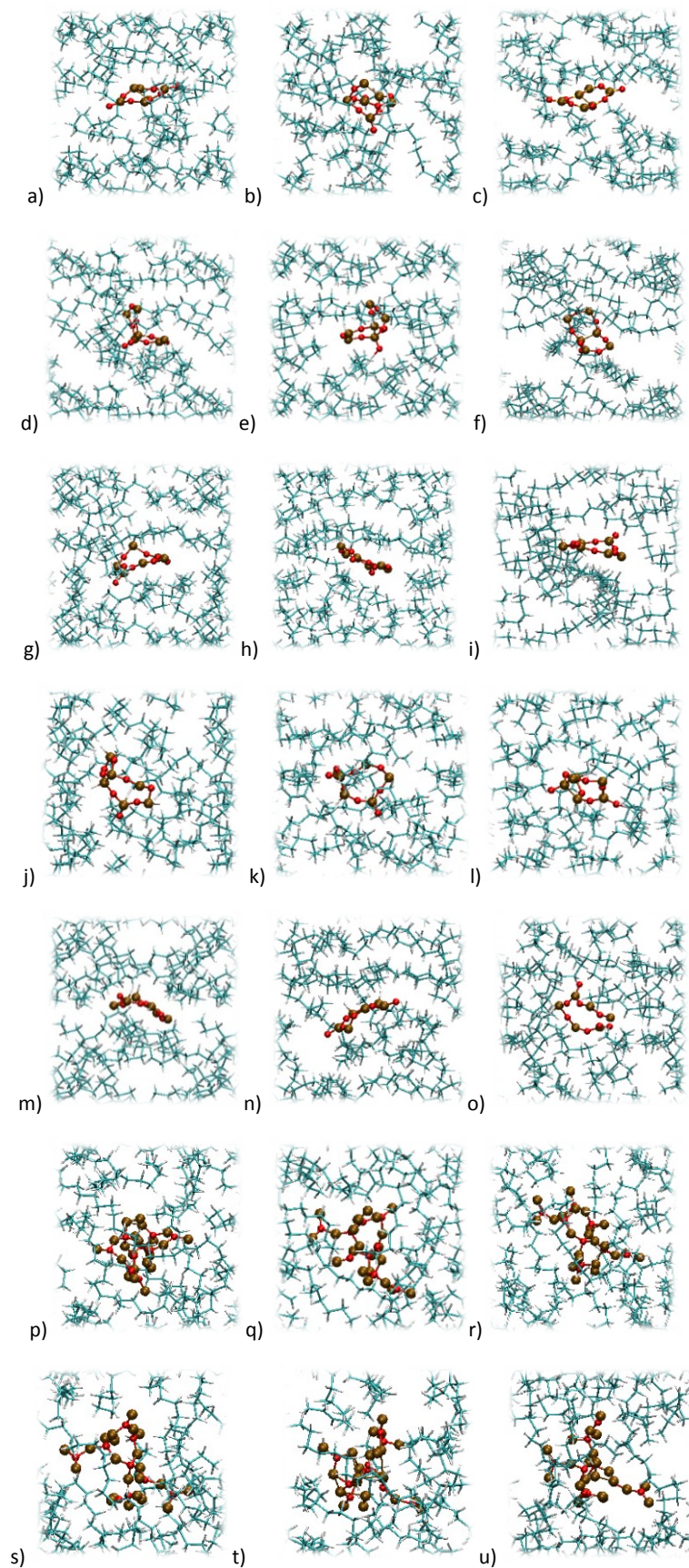


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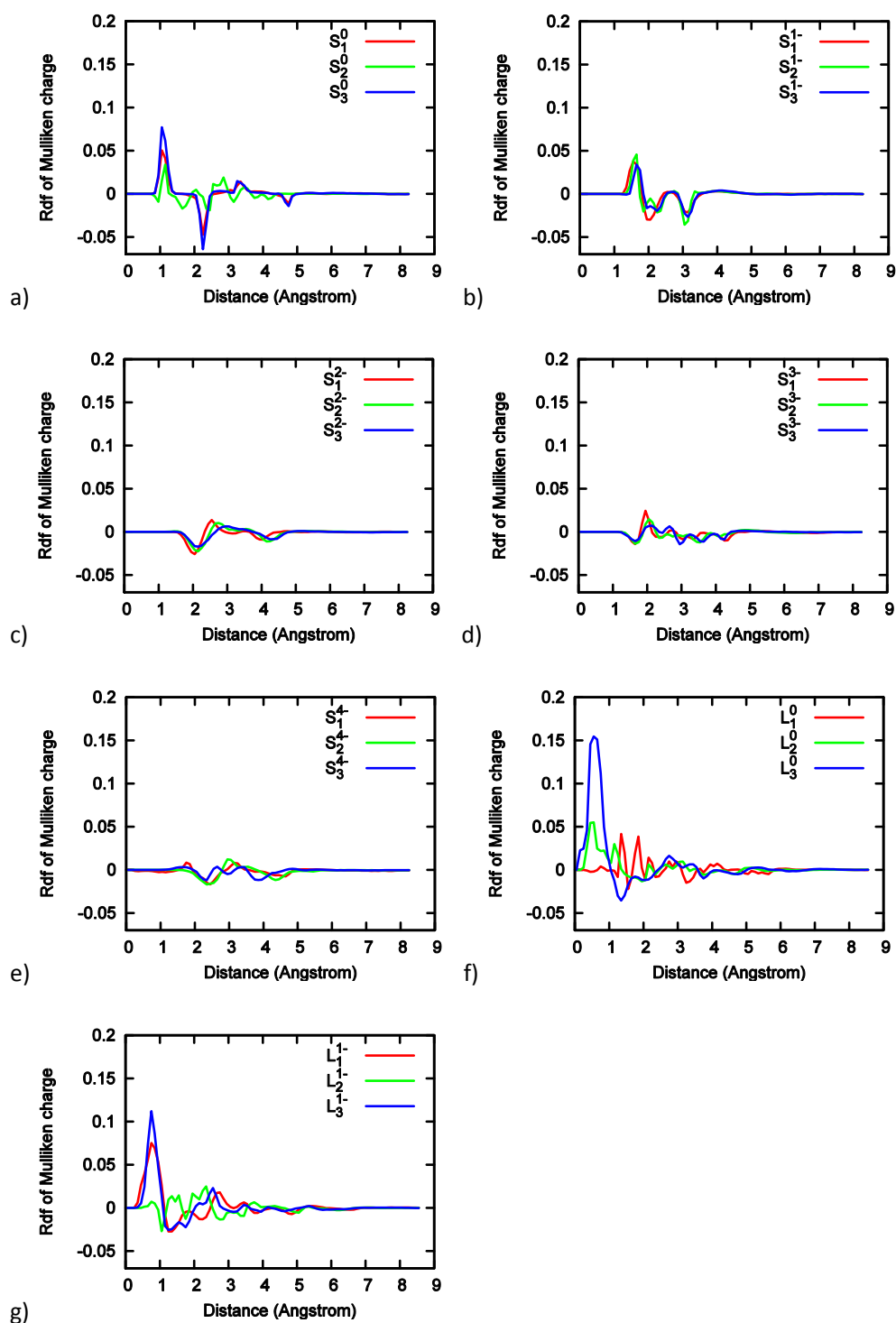


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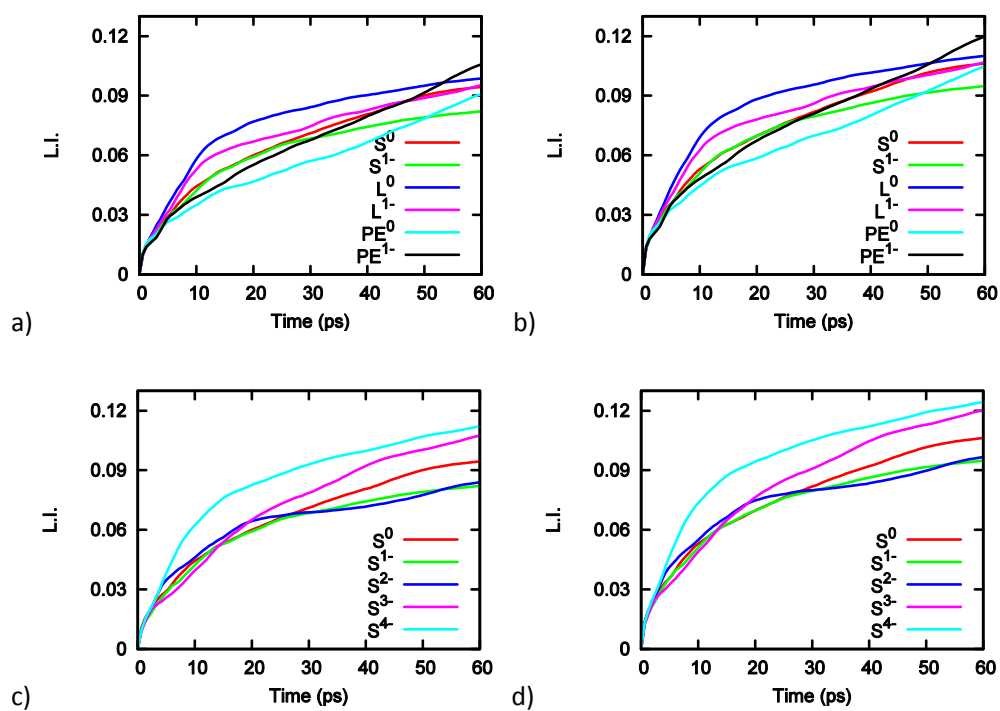


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