Atomistic Molecular Dynamics simulation study of a hybrid Poly (ethylene oxide) / Silica nanoparticle system

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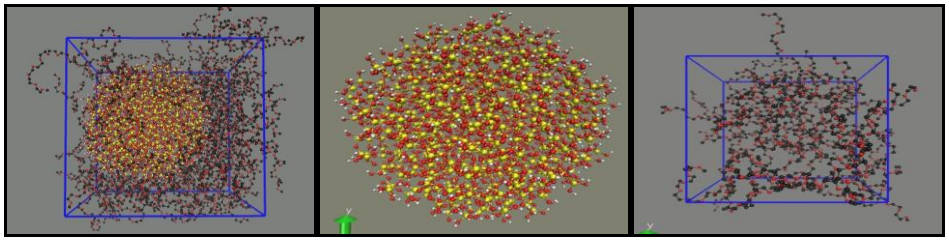
The goal of the present work is to study hybrid poly (ethylene oxide), PEO, silica nanoparticle systems. Poly (ethylene oxide), PEO, is a non-ionic, water - soluble, semi crystal polymer with many applications due to its flocculent, thickening, sustained-release, lubrication, dispersing and water-retention properties. Its hydrophilicity, biocompatibility, and versatility make it attractive as biomaterial as well. Additionally, PEO nanocomposites with non-crystalline nanoparticles are of important technological interest. [1-3]

In this work we perform detailed atomistic Molecular Dynamics simulations on a hybrid system of PEO with a Silica nanoparticle, in order to study and understand the structural and dynamical properties of the hybrid system. In more detail we directly calculate the density profile, chain conformations, segmental and terminal dynamics of PEO chains as a function of distance from the silica nanoparticle. [4-5] In a further step we will compare the simulation results to experimental data.



A) B) C)

Figure 1:A) Snapshot from a hybrid PEO/Silica nanoparticle system B) snapshot from a Silica nanoparticle C) snapshot from a PEO bulk

References

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