Properties of hybrid polymer/gold nanocomposite materials through a classical molecular dynamics approach.

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The properties of polyethylene chains around of a gold nanoparticle at a temperature of 450 K are investigated using a combination of density functional theory calculations and classical atomistic simulations. A classical Morse-type potential, used to describe the interaction between the polymer and the gold nanoparticle, was parameterized based on the results of density functional calculations [1]. Several gold nanoparticles with Wulff construction were studied, with diameter ranging from around 2.5-12 nm [2] and polyethylene chains consist of 22 monomers [3]. The structural, conformational, and dynamical properties of the chains were analyzed and compared to the behavior of the bulk polyethylene system. In more detail we report data concerning polymer density profiles, bond order parameter, segmental and terminal dynamics.

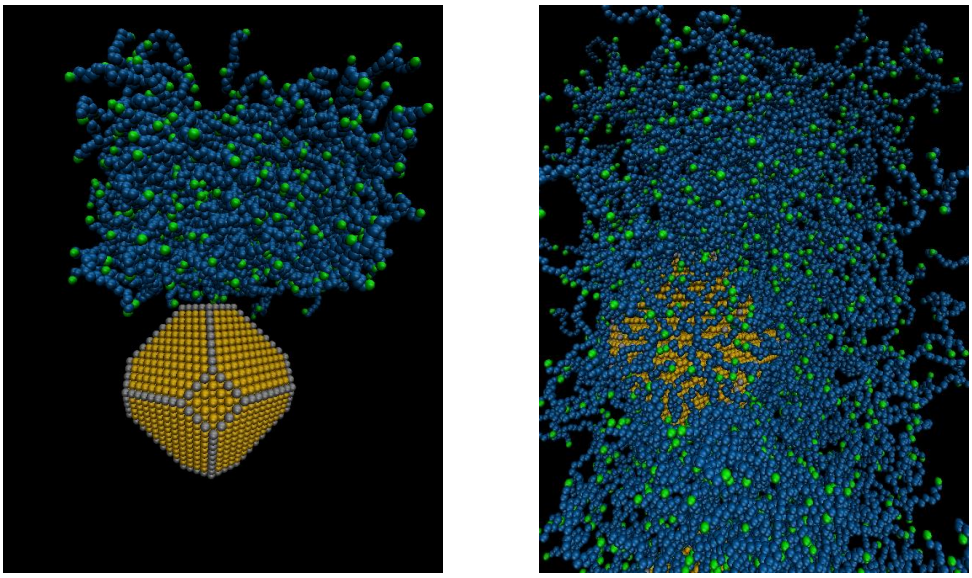

Figure 1: Snapshot from MD simulation of hybrid polyethylene/gold nanocomposite at 450K. Au nanoparticle (3101 atoms, diameter of 5.02 nm) and polyethylene (420 chains, 22-mers per chain) are shown. With yellow is the Au and with grey are the edges of Au nanoparticle. With blue are the CH_2 and with green the CH_3 monomers.

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References:

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