

## Supporting Information

# Unravelling the Effects of Size, Volume Fraction and Shape of Nanoparticle Additives on Crystallization of Nanocomposite Polymers

*Ahmad Jabbarzadeh<sup>1,2\*</sup> and Beny Halfina<sup>1</sup>*

Faculty of Engineering,

<sup>1</sup>School of Aerospace, Mechanical and Mechatronic Engineering,

<sup>2</sup>Sydney Nano Institute

The University of Sydney, NSW 2006, Australia

\*Corresponding author's email address: [ahmad.jabbarzadeh@sydney.edu.au](mailto:ahmad.jabbarzadeh@sydney.edu.au)

The following movies are provided as supporting material :

Movie 1:

Shows pure hexacontane ( $C_{60}H_{122}$ ) polymer crystallizes at a temperature of  $T=325K$  and  $P=1$  atm, during  $\sim 56$  ns of crystallization time. The movie is created from 600 individual frames. Frames are captured at 93 ps interval. Individual molecules are shown with different colours to improve clarity and detect molecular order and conformation, and formation of crystal lamella. The simulation includes 61400 united atoms.

Movie 2:

Nanocomposite hexacontane ( $C_{60}H_{122}$ ) system with a 4.5 nm cubic gold nanoparticle at the centre is shown during 56 ns of crystallization time conducted at  $T=325K$  and under the constant pressure of  $P=1$  atm. The nanocomposite system is created by mixing 87480 hexacontane united atoms and a 4.5 nm gold particle made of 4794 individual gold atoms at a volume fraction of 3.2 %.

Movie 3:

Isosurfaces of 90% crystallinity ( $g_2$ ) for pure hexacontane during 56 ns of crystallization. The results are made from snapshots taken at 470.9 ps time intervals.

Movie 4:

Isosurfaces of 90% crystallinity ( $g_2$ ) for nanocomposite gold hexacontane ( $C_{60}H_{122}$ ) during 56 ns of crystallization. The results are made from snapshots taken at 470.9 ps time intervals. The outline of the 4.5 nm cubic gold particle shown by blue colour is detected by isosurfaces of zero polymer density at the centre. The volume fraction of the nanocomposite system is  $\varphi=2.3\%$ .

Movie 5:

Isosurfaces of 90% crystallinity ( $g_2$ ) for nanocomposite gold hexacontane ( $C_{60}H_{122}$ ) during 56 ns of crystallization. The results are made from snapshots taken at 470.9 ps time intervals. The outline of the 5.5 nm spherical gold particle shown by blue colour is detected by isosurfaces of zero polymer density at the centre. The volume fraction of the nanocomposite system is  $\varphi=2.31\%$ .