Contribution ID: **563** Type: **Poster**

# Atomistic Molecular Dynamics Simulation of Graphene-isoprene Nanocomposites

*Monday, 21 May 2018 18:15 (15 minutes)*

Graphene-polymer nanocomposites have attracted some attentions from researchers recently due to its potential applications as a stress sensor or a lightweight-flexible conductor. A series of atomistic molecular dynamics simulations were performed for the systems consisting of a graphene flake within 4-mer isoprene matrix to assess the conformational order of isoprene molecules at the matrix-filler interphase. Two sizes (1.35 nm and 2.5 nm diameters) of graphene flakes were examined along with pure 4-mer isoprene melt. Local density and orientation of rubber polymer chains were measured as a function of distance from graphene. The interaction ranges between 4-mer isoprene and graphene, and between a pair of 4-mer isoprene chains were analyzed. These results provide some useful information for further research on rubber nanocomposites.

**Primary authors:** Dr CHANLERT, Purintorn (Program of Physics, Faculty of Science and Technology, Songkhla Rajabhat University); Dr SUTTHIBUTPONG, Thana (Department of Physics, Faculty of Science, King Mongkut University of Technology Thonburi); Dr WONG-EKKABUT, Jirasak (Department of Physics, Faculty of Science, Kasetsart University)

**Presenter:** Dr CHANLERT, Purintorn (Program of Physics, Faculty of Science and Technology, Songkhla Rajabhat University)

**Session Classification:** A05: Nanoscale and Surface (Poster)

**Track Classification:** Nanoscale Physics and Nanotechnology