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Study of the Mechanism how Carbon Nanoparticles Can Improve the Mechanical Properties of Natural Rubber using Multi-scale Molecular Dynamics Simulation

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Pure natural rubber (NR) has low durability and elasticity, which become a major bottleneck for practical use. To overcome the limitation, in general, the adding of carbon black and silica particles is applied[1,2], but carbon black has an effect of polymer cracking. Interestingly, the fullerene (C60) and carbon nanotube (CNT) can be used as rubber additive, resulting in the significant improvement of rubber mechanical properties as well as the thermal properties[3]. However, the mechanism of how the carbon nanoparticles reinforce rubber is still unclear. None of proper microscopic picture is provided to explain such filler reinforcement. Here, we study the molecular mechanism of how carbon nanoparticles improve the mechanical properties of NR. The atomistic and coarse-grained (CG) MD simulations are performed. The CG model of polyisoprene (the major component of NR) was developed based on MARTINI force field using "hybrid approach" which both structural and thermodynamic properties are used as a target during the parameterization. The advantages in time and length scales of CG modeling allow us to investigate the interactions between carbon nanoparticles in the NR at various concentrations and their size. The dispersion and aggregation of nanoparticles in the NR are expected to play an important role in improving mechanical properties of NR composite. The understanding of how C60 and CNT alter the physical NR properties is useful to produce more well-designed rubber composites preparation technique and develop rubber applications.

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Author: Dr KHUNTAWEE, Wasinee (1. Department of Physics, Faculty of Science, Kasetsart University, Bangkok, 10900, Thailand 2. Computational Biomodelling Laboratory for Agricultural Science and Technology (CBLAST), Faculty of Science, Kasetsart University, Bangkok 10900, Thailand)

Co-authors: Mr KITJANON, Jiramate (1. Department of Physics, Faculty of Science, Kasetsart University, Bangkok, 10900, Thailand 2. Computational Biomodelling Laboratory for Agricultural Science and Technology (CBLAST), Faculty of Science, Kasetsart University, Bangkok 10900, Thailand); Prof. WONG-EKKABUT, Jirasak (1.Department of Physics, Faculty of Science, Kasetsart University, Bangkok, 10900, Thailand 2.Computational Biomodelling Laboratory for Agricultural Science and Technology (CBLAST), Faculty of Science, Kasetsart University, Bangkok 10900, Thailand)

Presenter: Mr KITJANON, Jiramate (1. Department of Physics, Faculty of Science, Kasetsart University, Bangkok, 10900, Thailand 2. Computational Biomodelling Laboratory for Agricultural Science and Technology (CBLAST), Faculty of Science, Kasetsart University, Bangkok 10900, Thailand)

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