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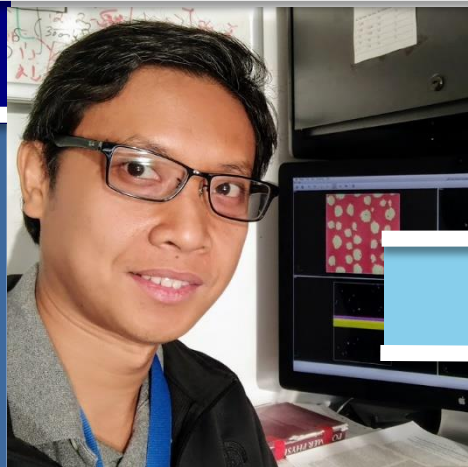1872

Dr. Jan-Michael Carrillo

"Coarse-Grained Molecular Dynamics Simulations of Soft Matter Systems"

Oak Ridge National Laboratory (ORNL)

Center for Nanophase Materials Sciences and Computational Sciences and Engineering Division

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Abstract: Soft matter broadly refers to a class of materials that are structurally altered by external stresses comparable with thermal energy. The understanding of these systems, usually composed of macromolecules such as polymers, proteins and lipids, is particularly challenging because of their vast degrees of freedom, where typically the molecular scale does not directly translate to the macroscopic (experiment) scale due to self-organization of the constituent macromolecules in the mesoscale. In this talk, I will present my recent work in the area, highlighting my close collaboration with neutron scattering experiments, material synthesis and characterization. Here, I used large-scale coarse-grained molecular dynamics simulations and existing theoretical models to interpret the simulation results. The eventual goals of these simulations are to provide insights to help in the interpretation of past experiments and offer guidance in designing future experiments.

Bio (cont.): In 2015, Dr. Carrillo transitioned into a research scientist staff position in the Joint Institute for Computational Sciences, which is a joint institute between ORNL and the University of Tennessee (UTK), where he maintains close collaborations with researchers affiliated with both institutions. These collaborations involve performing large-scale molecular dynamics simulations of soft matter systems, such as polymers having different architectures and lipid bilayer membranes, and are complementary to experiments performed at ORNL.

Bio: Dr. Jan-Michael Carrillo received his Ph.D. in Polymer Science in 2009 from the Institute of Materials Science at the University of Connecticut (UConn). After which, he did postdoctoral trainings at the Physics Department of UConn and then at the Oak Ridge Leadership Computing Facility (OLCF) in Oak Ridge National Laboratory (ORNL).

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