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Simulation of Self-Assembly of Functionalized Silsesquioxane Molecules JOHN KIEFFER, FENG QI, JINHUA ZHOU, University of Michigan, MURAT DURANDURDU, University of Texas - El Paso, XI ZHANG, SHARON GLOTZER, University of Michigan, CHENG-YING LEE, MATT NEUROCK, University of Virginia — We have developed a computational framework for the simulation of structural assembly in Polyhedral oligomeric silsesquioxane (POSS) nanocomposites, by combining computational techniques ranging from ab initio quantum mechanical calculations to molecular dynamics simulations to coarse-grained mesoscale modeling methods. Using ab initio calculations we predict the inherent properties of molecular building blocks. Using large- scale molecular dynamics simulations we reproduce the transport, reaction, and microphase evolution processes that occur during nano-assembly, and thereby generate realistic models that serve to establish structure-property-processing relationships for these materials. In this presentation the general approach taken with our the computational framework will be outlined and results from two representative materials simulation studies will be discussed. One example details the strategies pursued for the design of materials with photonic applications. The other one describes the peculiar amphiphilic behavior of monotethered POSS that causes nano-phase separation and can be exploited for pattern formation at this scale.

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