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Cloud computing in nanoHUB powering education and research

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ABSTRACT

The lack of easy access to powerful simulations and lack of a workforce trained on computer simulations of materials are important factors limiting the adoption of ICME in industry. NSF's nanoHUB.org is a web-portal that enables users to perform online simulations using simply a web browser. With over 300 simulation tools freely available and high-quality online training and educational material, nanoHUB.org can play an important role making simulation tools widely accessible and training a new generation of engineers familiar with ICME tools. In this presentation, we describe PolymerModeler, a nanoHUB.org tool that offers a free platform for research and education in atomistic polymer simulations. The tool allows users to construct and visualize atomistic models of thermoplastic polymers. The mechanical properties of the resulting systems may be studied using LAMMPS, within the PolymerModeler tool. LAMMPS simulations run on NSF-funded HPC resources, and the results display in the web browser. Users do not need to download or install any software. A first time user guide introduces the tool and common usage scenarios. The polymer builder section of the tool constructs chains by adding successive monomers. Several prebuilt monomers are available, and users can upload any repeated unit, in PDB or XYZ format, making it a very general amorphous builder.