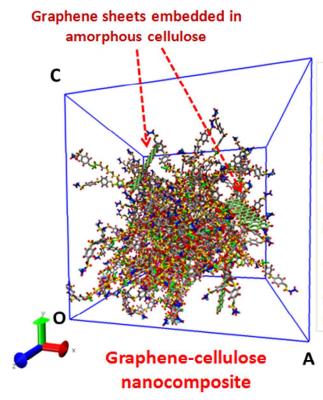
Molecular Dynamics Simulation and Characterization of Graphene-Cellulose Nanocomposites

R. Rahman[†], J. T. Foster^{\dagger , ¥} and A. Haque^{¶*}

[†]Center for Simulation, Visualization and Real-Time Prediction (SiViRT), The University of Texas and San Antonio, San Antonio, TX 78249. [¥]Department of Mechanical Engineering, The University of Texas and San Antonio, San Antonio, TX 78249.

[¶]Department of Aerospace Engineering and Mechanics, The University of Alabama, Tuscaloosa, AL 35401.



Research highlights

•Adding 1%-3% graphene enhances the Young's modulus of graphene-cellulose nanocomposites significantly.

•Dispersed graphenes in cellulose lead to better stiffness.

•Graphene with larger aspect ratio has stronger non-bonded interaction with cellulose at the graphene-cellulose interface.