

Abstract Submitted
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Molecular Study of Charge Transport at the Interface between Nanostructures and Matrix in Nanocomposites¹ PEDRO DEROSA, Louisiana Tech/Grambling State, DAVID COSSEY, JACQUELYN HOYLE, Louisiana Tech University, LA TECH TEAM — The insertion of nanostructures in a polymer matrix has opened up a myriad of possibilities for multifunctional materials. The number of opportunities is however as large as the challenges involved in the study of these materials. One of those challenges, and the focus of this work, is the nature of the interface between the matrix and the nanoinsert and how this affects important properties such electrical transport. Particularly, it has been acknowledge for CNT-polymer composites that conductivity is significant at CNT concentrations below the percolation limit owing this conductivity to tunneling transport from CNT to CNT through the polymer matrices. In this work we described a set of calculations showing that parameters that are relevant to tunneling transport can be calculated from molecular models, namely Density Functional Theory and Green's Functions. In addition, a preliminary study relevant to heat transport at the interface will be described, particularly heat generated by currents and the interface will be focused.

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