

Abstract Submitted
for the 4CS21 Meeting of
The American Physical Society

Assessment of Material Properties of Carbon Nanotubes(CNTs) and C60 Fullerenes(C60HyFn) with PVC Derivatives as Potential Conductive Pipes SIENA LEE, RISE-NJ, RISE-NJ TEAM — This study represents a discovery of Carbon Nanotubes(CNTs) and C60 Fullerenes(C60HyFn) with polymers such as PVC derivatives. Electron donoracceptor (D-A) energy transfer-based strategies were employed to construct functionalized conductive complexes using computer simulations. Upon interaction with P3HT, unique electrochemical properties were shown due to highly efficient D-A energy transfer from the polymers to the CNTs or C60. Polymers act as electron donors and hydrophobic CNTs or fullerenes act as an electron acceptor, enabling the production of applications in environmentally friendly electronic devices. This research performed the investigation of the interaction of CNTs and fullerenes with polymers to find their properties and efficiencies in conductivity. Fullerenes were studied as the conducting layer in an aqueous-processed conductive device and the relative angular orientation between the P3HT and PCBM was considered in finding the stability and the total energy of the complex. Molecular dynamics (MD) and quantum mechanics approaches such as the Density Functional Theory(DFT) were used to study the behavior.

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Date submitted: 17 Sep 2021

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