Jayamurugan, G.; Vasu, K. S.; Rajesh, Y. B. R. D.; Suhas, K.; Maiti, P. K.; Sood, A. K.; Jayaraman, N., 2011, "Wrapping single-walled carbon nanotubes with a native poly(propyl ether imine) dendrimers: fluoroscence quenching, electrical transport, Raman experiments and molecular dynamics simulations" *J. Chem. Phys*., *134*, 104507/1 – 104507/6.

In this communication, we report results of a study of the interaction of single-walled carbon nanotube with non-toxic, un-derivatized and native poly(ether imine) dendrimers. These two unrelated nanomaterials are considered as versatile platforms in a variety of studies and possible applications on their own merits, yet exploring the interactions between these two specific platforms is un-known currently. We identify that charge-transfer and hydrophobic interactions mediate a stable complexation between the dendrimer and nanotubes, through fluorescence and Raman spectroscopies, electrical conductivities and molecular dynamics simulations. Inherent fluorescence of the dendrimer is used a tool to follow the complexation, wherein quenching of fluorescence occurs upon nanotube complexation. Following this, changes in the Raman spectral modes, and electrical conductivities of nanotube due to dendrimer complexation were assessed, thereby ascertaining the nature of interactions. Subsequently, efforts were undertaken to study the complexations through fully-atomistic molecular dynamics simulations, allowing to corroborate the experimental studies. The oxygen and nitrogen moieties constituting the dendrimer, not only form the basis of inherent dendrimer fluorescence, but also undergo charge-transfer interactions with nanotubes, wherein a quenching of fluorescence occurs. Such a study utilizing the inherent fluorescence of a dendrimer as a tool to monitor their complexation with nanotubes is un-known currently. Details associated with the effect of pH on complexation have also been assessed, in both experiment and computation. The novelty of the work relies on the demonstration of non-covalent functionalization of SWNT with a native, un-derivatized dendrimer, whose inherent properties not only allow monitoring the complexation process, which is hitherto un-known, but also offer a biologically-benign potential to the complex, when compared to SWNT alone.