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Effect of Polymer Conformation on Wrapping with Carbon Nanotubes[1]

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We have employed first-principles density-functional calculations for investigating the effect of polymer conformations on the helical wrapping of carbon nanotubes and the selective enhancement of individual carbon nanotubes. Our attention is directed to the electronic structure effects associated with the polymer conformations. The calculation results are compared with the experimental investigations of using poly[(*p*-phenylenevinylene)-*co*-(*p*- phenyleneethynylene)] (PPE/PPV) for selecting specific single- walled carbon nanotubes.

[1]In collaboration with Xiao-Qian Wang, Clark Atlanta University.