First-Principles Optoelectronic Properties of Quasi-One-Dimensional Nanostructured Materials

John W. Mintmire, Thushari Jayasekera, and Junwen Li
Department of Physics
Oklahoma State University
Stillwater, OK 74078

One major approach for efficient polymeric photovoltaic materials lies in the use of bulk heterojunctions, which mix two different organic polymeric materials which act as donor and acceptor semiconductors. In these bulk heterojunctions the donor polymer typically acts as the light absorber, creating an electron-hole pair and then donating the excited electron to the acceptor polymer. A deep theoretical understanding of the physical process at work in these materials will require a knowledge of the electron states near the Fermi level for both the donor and acceptor. Recent reports by Kymakis, et al. suggest that mixtures of single wall carbon nanotubes (SWNT) and poly-3-octylthiophene (P3OT) represent an alternative class of organic semiconducting materials that can be used to manufacture organic photovoltaic cells with improved performance. In addition, Lieber, at al. have recently reported the synthesis of coaxial silicon nanowires with possible application as photovoltaic devices. We discuss our first-principles simulations on the geometry optimization and calculated electronic properties of several quasi-one-dimensional materials with potential application as photovoltaics.

This work was supported by the US Department of Energy through the DOE EPSCoR National Laboratory Partnership program. (Grant DE-FG02-07ER46362)