**Documentation of Atomistic Models, Force Field Files, and Script**

This folder contains the following files:

**1) Atomistic models in car/mdf format for use with Materials Studio, visualization with VMD, and other programs**

1 nm CNT, 2 nm CNT, 3 nm CNT, 4 nm CNT, composite with PAN 50% aligned and a 1 nm CNT, polyacrylonitrile (PAN) oligomer (only 20 repeat units)

The models contain the atomic coordinates, as well as atomic charges and force field types ready for simulations using Discover, Forcite, and LAMMPS (after conversion from Materials Studio format to LAMMPS format using the msi2lmp program). The models are this simulation-ready. When using other programs, the files can also be used, however, atomic charges and atom types may have to be assigned manually, and the PCFF force field parameters imported.

**2) Force field file in .frc format**

The file pcff\_iff\_v1\_5\_CNT\_poly\_solv.frc contains all force field parameters. For use in Materials Studio, import both the .frc and \_templates.dat file.

**3) Matlab script to calculate energy surface**

This script can be used or modified to calculate the energy surfaces (see Figure S3 in the Supporting Information)