A software module that models the electronic and mechanical aspects of hydrocarbon molecules and carbon molecular structures on the basis of first principles has been written for incorporation into, and execution within, the Easy (Modular) Tight-Binding (EZTB) software infrastructure, which is summarized briefly in the immediately preceding article. Of particular interest, this module can model carbon crystals and nanotubes characterized by various coordinates and containing defects, without need to adjust parameters of the physical model.

The module has been used to study the changes in electronic properties of carbon nanotubes, caused by bending of the nanotubes, for potential utility as the basis of a nonvolatile, electric-charge-free memory devices. For example, in one application of the module, it was found that an initially 50-nm-long carbon, (10,10)-chirality nanotube, which is a metallic conductor when straight, becomes a semiconductor with an energy gap of ≈3 meV when bent to a lateral displacement of 4 nm at the middle.

This program was written by Seungwon Lee and Paul von Allmen of Caltech for NASA’s Jet Propulsion Laboratory.

This software is available for commercial licensing. Please contact Karina Edmonds of the California Institute of Technology at (626) 395-2322. Refer to NPO-44781.