

Geometric and electronic structures of nanocarbon hybrid materials

Okada Susumu

University of Tsukuba

Contact e-mail: *sokada@comas.frsc.tsukuba.ac.jp*

Hybrid structures of nanocarbon materials with foreign materials usually exhibits interesting variations arising from dimensionality of constituents, interunit spacing, and structural hierarchy. In the present paper, we will discuss the geometric and electronic structures of various nanocarbon hybrid structures consisting of fullerenes, nanotubes, and graphene using the first-principles total-energy calculation based on density functional theory.