Abstract
First, the Thomas–Fermi–Amaldi (TFA) equation was formulated with a newly-derived condition to remove the singularities at the nuclei, coincided with the molecular cusp condition. Next, the collocation method was applied to the TFA equation using the grid-based density functional theory. In this paper, the electron densities and the radial probabilities for specific atoms (He, Be, Ne, Mg, Ar, Ca) were found to agree with those from Thomas–Fermi–Dirac (TFD) method. Total energies for specific atoms (He, Ne, Ar, Kr, Xe, Rn) and molecules (H₂, CH₄) were also found to be close to those from the Hartree–Fock method using the Pople basis set 6-311G relatively to TFD method. In addition, the computational expense to determine the electron density and its corresponding energy for a large scale structure, such as a carbon nanotube, is shown to be much more efficient compared to the conventional Hartree–Fock method using the 6–31G Pople basis set.